**Supporting Information.**

**Table I.** NMR chemical shifts of the alkaline form of *S. cerevisiae* cytochrome *c* in 50 mM phosphate buffer + NaOH, pH 11.1, T=298 K. The shifts of the axial ligands to the iron are written in bold.

| residue | N | HN | α | | β | | others |
|---|---|---|---|---|---|---|---|
| THR-5 | | | | | | | |
| GLU-4 | | | | | | | |
| PHE-3 | 125.10 | 8.60 | 4.24 | | 1.44 | | δ 6.95; ε 7.32 |
| LYS-2 | 119.61 | 7.05 | | | | | |
| ALA-1 | | | | | | | |
| GLY 1 | | | | | | | |
| SER 2 | | | | | | | |
| ALA 3 | | | | | | | |
| LYS 4 | | | | | | | |
| LYS 5 | | | | | | | |
| GLY 6 | | | | | | | |
| ALA 7 | | | | | | | |
| THR 8 | | | | | | | |
| LEU 9 | 124.09 | 7.92 | 4.02 | | 2.16 | 1.71 | γ 1.30; δ 1.10, δ 0.87 |
| PHE 10 | 120.30 | 8.80 | 3.93 | | 2.89 | | δ 7.03; ε 6.12; ζ 8.62 |
| LYS 11 | 120.30 | 8.24 | 3.17 | | 1.92 | | γ 1.20, 1.07; δ 0.73, 0.54 |
| THR 12 | 107.22 | 7.93 | 4.27 | | 3.95 | | γ 1.29 |
| ARG 13 | 116.83 | 8.55 | 5.06 | | 2.20 | 2.09 | γ 2.50 |
| CYS 14 | 115.18 | 7.99 | 5.18 | | 1.73 | 0.84 | |
| LEU 15 | 121.37 | 7.18 | 3.95 | | | | δ 1.72, 1.28 |
| GLN 16 | 124.18 | 10.71 | 3.87 | | 2.02 | 1.84 | γ 3.06, 2.72; Hε 7.71, 7.36; Nε 114.80 |
| CYS 17 | 113.08 | 8.98 | 5.79 | | 2.01 | | |
| **HIS 18** | **120.66** | **11.40** | **10.80** | | **15.37** | **9.74** | **δ1 13.8, δ2 21.0; ε1 -10.2** |
| THR 19 | 111.70 | 11.13 | 6.51 | | 5.63 | | γ 2.39 |
| VAL 20 | | 8.29 | 5.00 | | | | |
| GLU 21 | | 9.08 | | | | | |
| LYS 22 | | | | | | | |
| GLY 23 | | | | | | | |
| GLY 24 | 108.26 | 8.19 | 4.5 | 3.81 | | | |
| PRO 25 | - | | | | | | |
| HIS 26 | | | | | | | |
| LYS 27 | | | | | | | |
| VAL 28 | | | | | | | |
| GLY 29 | 104.13 | 8.70 | -1.25 | 0.79 | | | |
| PRO 30 | - | | 5.78 | | | | γ 0.40, -0.051; δ –4.37, -1.76 |
| ASN 31 | | | 6.72 | | | | Hδ 9.08, 8.27; Nδ 115.31 |
| LEU 32 | 123.05 | 10.11 | 4.84 | | 2.42 | 1.64 | δ 0.84, -0.45 |
| HIS 33 | 119.96 | 8.30 | 3.93 | | 3.27 | 3.12 | |
| GLY 34 | | | 3.81 | 3.68 | | | |
| ILE 35 | 116.82 | 7.14 | 3.59 | | 1.56 | | γ-$CH_3$ –0.13; γ 0.75,0.64; δ 0.17 |
| PHE 36 | 115.56 | 7.84 | 4.15 | | 2.86 | | δ 7.12; ε 6.68; ζ 7.00 |
| GLY 37 | 109.70 | 8.69 | 4.15 | 3.63 | | | |
| ARG 38 | 121.37 | 8.03 | 4.53 | | 2.10 | 1.84 | γ 1.69; δ 1.92 |
| HIS 39 | 118.25 | 7.76 | 5.35 | | 2.74 | 2.58 | δ1 6.50 |
| SER 40 | 115.49 | 8.63 | 4.82 | | 4.24 | 4.22 | |
| GLY 41 | 112.75 | 8.13 | 1.22 | 3.33 | | | |
| GLN 42 | 113.38 | 7.65 | 3.82 | | | | |
| ALA 43 | 127.87 | 7.85 | 4.34 | | 1.67 | | |
| GLU 44 | | 8.44 | 4.61 | | | | |
| GLY 45 | 112.43 | 9.99 | 4.34 | 4.90 | | | |
| TYR 46 | | 6.62 | 3.75 | | 1.71 | | δ 7.04, 7.31; ε 6.93, 6.24 |

| | | | | | | |
|---|---|---|---|---|---|---|
| SER 47 | | | | | | |
| TYR 48 | | | | 2.08 | | δ 6.15; ε 6.73 |
| THR 49 | | 9.42 | | | | γ 1.35 |
| ASP 50 | | | | | | |
| ALA 51 | | | | | | |
| ASN 52 | 118.63 | 8.16 | 4.03 | 2.97 | 2.89 | δN 106.55; δNH 8.70, 7.19 |
| ILE 53 | 119.95 | 7.59 | 3.27 | 1.76 | | γ 0.95, 1.05; δ 0.82 |
| LYS 54 | 118.66 | 8.95 | 3.79 | 1.73 | 1.62 | γ 1.35 |
| LYS 55 | 119.22 | 7.33 | 3.72 | 1.65 | | γ 1.20; δ 0.93 |
| ASN 56 | 114.45 | 8.16 | 4.36 | | | |
| VAL 57 | 115.14 | 7.23 | 3.66 | 0.97 | | γ -0.35, 0.28 |
| LEU 58 | 127.87 | 8.12 | 3.66 | 1.48 | 0.71 | γ 0.94; δ 0.57, 0.13 |
| TRP 59 | 128.90 | 7.93 | 4.89 | | | δ1 6.93; ε 7.50 εNH 8.88; Nε 121.00; |
| | | | | 3.66 | 2.53 | ξ 6.55, 7.02; η 5.60 |
| ASP 60 | 125.12 | 9.65 | | | | |
| GLU 61 | | | | | | |
| ASN 62 | 126.15 | 7.63 | 4.47 | 2.94 | 1.85 | |
| ASN 63 | 122.71 | 9.40 | 4.43 | 3.00 | 2.77 | δ 6.86, 6.64 |
| MET 64 | 123.40 | 8.58 | 4.02 | 1.60 | 1.32 | ε -0.89 |
| SER 65 | 114.11 | 7.32 | 3.44 | 3.99 | 3.74 | |
| GLU 66 | 120.30 | 7.68 | 3.69 | 1.85 | 1.67 | γ 2.17 |
| TYR 67 | 121.04 | 8.30 | 3.43 | 2.98 | 2.90 | |
| LEU 68 | 111.33 | 8.22 | 2.90 | 1.92 | 1.64 | γ 1.02; δ 0.03 |
| THR 69 | 115.56 | 7.25 | 3.77 | 4.05 | | γ 1.09 |
| ASN 70 | 107.22 | 6.09 | 4.06 | 2.93 | 2.64 | |
| PRO 71 | - | | | 0.08 | | γ 0.60; δ 1.09 |
| ALA 72 | 112.83 | 7.82 | | | | |
| **LYS 73** | **122.29** | **8.19** | **5.06** | **10.94** | **9.43** | **γ 6.7, δ 24.5** |
| TYR 74 | | | | | | |
| ILE 75 | 121.35 | 7.68 | 3.86 | 2.22 | | γ-$CH_2$ 1.15, 0.28; γ-$CH_3$ -0.73; δ -0.99 |
| PRO 76 | - | | | | | |
| GLY 77 | | 8.27 | | | | |
| THR 78 | | 8.63 | | | | |
| ALA 79 | 125.12 | 7.97 | 2.36 | 1.12 | | |
| MET 80 | 112.39 | 6.92 | 4.15 | | | γ 1.89, 1.41 |
| ALA 81 | 115.48 | 6.44 | 3.51 | 0.67 | | |
| PHE 82 | | | | 1.93 | | δ 6.87; ε 7.02; ξ 6.86 |
| GLY 83 | 108.26 | 9.53 | | | | |
| GLY 84 | 105.50 | 7.54 | 3.51 | | | |
| LEU 85 | 116.46 | 7.80 | 4.08 | 1.52 | 0.97 | γ 1.08; δ 0.00 |
| LYS 86 | 119.15 | 8.39 | 4.21 | | | γ 1.10; δ 0.27, -0.03 |
| LYS 87 | 120.30 | 7.99 | 3.59 | 2.39 | 2.27 | γ 1.04; δ 1.17 |
| GLU 88 | | | | | | |
| LYS 89 | | | | | | |
| ASP 90 | 115.55 | 6.37 | 4.28 | 2.86 | 2.52 | |
| ARG 91 | 117.90 | 7.48 | 3.79 | 1.80 | 1.59 | γ 1.04 |
| ASN 92 | 117.56 | 8.70 | 4.62 | 2.71 | | |
| ASP 93 | 125.09 | 8.67 | 4.19 | 2.65 | | |
| LEU 94 | 120.30 | 8.55 | 4.21 | 2.12 | 1.90 | γ 1.08; δ 1.38 |
| ILE 95 | 119.95 | 9.12 | 3.60 | 2.07 | | γ 0.08; γ$CH_3$ 0.98; δ 0.53 |
| THR 96 | 117.20 | 8.15 | 3.78 | 4.39 | | γ 1.18 |
| TYR 97 | 119.55 | 7.81 | 4.08 | 3.54 | 3.09 | |
| LEU 98 | 119.94 | 9.34 | 3.33 | 1.95 | 1.89 | γ 1.61; δ 0.79, -0.11 |
| LYS 99 | 120.66 | 8.67 | 3.41 | 1.90 | 1.43 | γ 0.47; δ 0.83 |
| LYS 100 | 115.83 | 6.56 | 4.06 | 1.70 | | γ 1.30 |
| ALA 101 | 119.61 | 8.33 | 3.80 | 0.46 | | |
| SER 102 | 102.41 | 7.26 | 4.30 | | | γ 0.81 |
| GLU 103 | 125.80 | 6.65 | 3.93 | 2.16 | 1.87 | γ 2.71 |

Heme protons chemical shifts (ppm)

| | |
|---|---|
| $2^1CH_3$ | 14.19 |
| $3^1CH$ | -0.82 |
| $3^2CH_3$ | -2.25 |
| $7^1CH_3$ | 12.11 |
| $8^1CH$ | 1.15 |
| $8^2CH_3$ | -0.017 |
| $12^1CH_3$ | 19.56 |
| $18^1CH_3$ | 25.63 |

**Table II.** Pseudocontact shifts for the alkaline form of S. cerevisiae cyt c K79A, calculated by subtracting the chemical shift of the reduced native protein from the chemical shifts of the alkaline form.

| res. num. | res.nam. | atom nam. | pcs | multiplicity | tolerance |
|---|---|---|---|---|---|
| 3 | PHE | HN | -0.285 | 1 | 0.5 |
| 3 | PHE | HA | -0.248 | 1 | 0.3 |
| 3 | PHE | HD1 | -0.195 | 2 | 0.3 |
| 3 | PHE | HD2 | -0.195 | 2 | 0.3 |
| 3 | PHE | HE1 | -0.106 | 2 | 0.3 |
| 3 | PHE | HE2 | -0.106 | 2 | 0.3 |
| 4 | LYS | HN | 0.305 | 1 | 0.5 |
| 14 | LEU | HN | -0.173 | 1 | 0.5 |
| 14 | LEU | HA | -0.158 | 1 | 0.3 |
| 14 | LEU | HG | -0.551 | 1 | 0.3 |
| 15 | PHE | HN | -0.158 | 1 | 0.5 |
| 15 | PHE | HA | -0.199 | 1 | 0.3 |
| 15 | PHE | HZ | 2.45 | 1 | 0.3 |
| 15 | PHE | HD1 | -0.153 | 2 | 0.3 |
| 15 | PHE | HD2 | -0.153 | 2 | 0.3 |
| 16 | LYS | HN | -0.149 | 1 | 0.5 |
| 16 | LYS | HA | -0.911 | 1 | 0.8 |
| 16 | LYS | HG3 | -0.25 | 1 | 0.3 |
| 17 | THR | HN | -0.151 | 1 | 0.5 |
| 17 | THR | HA | -0.144 | 1 | 0.3 |
| 17 | THR | HG21 | -0.139 | 3 | 0.3 |
| 17 | THR | HG22 | -0.139 | 3 | 0.3 |
| 17 | THR | HG23 | -0.139 | 3 | 0.3 |
| 18 | ARG | HN | -0.154 | 1 | 0.5 |
| 18 | ARG | HA | -0.144 | 1 | 0.3 |
| 20 | LEU | HN | -0.194 | 1 | 0.5 |
| 21 | GLN | HA | -0.097 | 1 | 0.3 |
| 24 | THR | HN | 3.786 | 1 | 0.8 |
| 24 | THR | HA | 1.976 | 1 | 0.3 |
| 24 | THR | HB | 1.268 | 1 | 0.3 |
| 24 | THR | HG21 | 1.348 | 3 | 0.3 |
| 24 | THR | HG22 | 1.348 | 3 | 0.3 |
| 24 | THR | HG23 | 1.348 | 3 | 0.3 |
| 29 | GLY | HN | 0.295 | 1 | 0.5 |
| 34 | GLY | HN | 0.938 | 1 | 0.5 |
| 35 | PRO | HA | 2.154 | 1 | 0.8 |
| 36 | ASN | HN | 0.93 | 1 | 0.5 |
| 36 | ASN | HA | 2.656 | 1 | 0.8 |
| 37 | LEU | HN | 2.207 | 1 | 0.8 |
| 37 | LEU | HA | 0.926 | 1 | 0.8 |
| 38 | HIS | HN | 0.751 | 1 | 0.5 |
| 38 | HIS | HA | 0.045 | 1 | 0.3 |
| 40 | ILE | HN | 0.039 | 1 | 0.5 |
| 40 | ILE | HA | -0.142 | 1 | 0.3 |
| 40 | ILE | HB | -0.05 | 1 | 0.3 |
| 41 | PHE | HN | 0.001 | 1 | 0.5 |

| | | | | | |
|---|---|---|---|---|---|
| 41 | PHE | HA | -0.234 | 1 | 0.3 |
| 41 | PHE | HZ | -0.11 | 1 | 0.3 |
| 41 | PHE | HD1 | -0.108 | 2 | 0.3 |
| 41 | PHE | HD2 | -0.108 | 2 | 0.3 |
| 41 | PHE | HE1 | -0.151 | 2 | 0.3 |
| 41 | PHE | HE2 | -0.151 | 2 | 0.3 |
| 42 | GLY | HN | -0.094 | 1 | 0.5 |
| 43 | ARG | HN | -0.041 | 1 | 0.5 |
| 43 | ARG | HA | -0.322 | 1 | 0.3 |
| 44 | HIS | HN | -0.202 | 1 | 0.5 |
| 44 | HIS | HA | -0.213 | 1 | 0.3 |
| 45 | SER | HN | -0.15 | 1 | 0.5 |
| 45 | SER | HA | -0.177 | 1 | 0.3 |
| 46 | GLY | HN | -0.107 | 1 | 0.5 |
| 47 | GLN | HN | -0.593 | 1 | 0.5 |
| 47 | GLN | HA | -0.833 | 1 | 0.3 |
| 48 | ALA | HN | -0.83 | 1 | 0.5 |
| 48 | ALA | HA | -0.072 | 1 | 0.3 |
| 48 | ALA | HB1 | 0.104 | 3 | 0.3 |
| 48 | ALA | HB2 | 0.104 | 3 | 0.3 |
| 48 | ALA | HB3 | 0.104 | 3 | 0.3 |
| 49 | GLU | HN | -0.388 | 1 | 0.5 |
| 49 | GLU | HA | 0.349 | 1 | 0.3 |
| 51 | TYR | HN | -0.892 | 1 | 0.5 |
| 51 | TYR | HA | -0.373 | 1 | 0.3 |
| 54 | THR | HN | -1.091 | 1 | 0.5 |
| 54 | THR | HG21 | -0.467 | 3 | 0.3 |
| 54 | THR | HG22 | -0.467 | 3 | 0.3 |
| 54 | THR | HG23 | -0.467 | 3 | 0.3 |
| 56 | ALA | HB1 | 0.104 | 3 | 0.3 |
| 56 | ALA | HB2 | 0.104 | 3 | 0.3 |
| 56 | ALA | HB3 | 0.104 | 3 | 0.3 |
| 57 | ASN | HN | -0.107 | 1 | 0.5 |
| 57 | ASN | HA | -0.146 | 1 | 0.3 |
| 58 | ILE | HN | -0.103 | 1 | 0.5 |
| 58 | ILE | HA | -0.146 | 1 | 0.3 |
| 58 | ILE | HB | -0.126 | 1 | 0.3 |
| 58 | ILE | HG21 | 0.091 | 3 | 0.3 |
| 58 | ILE | HG22 | 0.091 | 3 | 0.3 |
| 58 | ILE | HG23 | 0.091 | 3 | 0.3 |
| 58 | ILE | HD11 | -0.275 | 3 | 0.3 |
| 58 | ILE | HD12 | -0.275 | 3 | 0.3 |
| 58 | ILE | HD13 | -0.275 | 3 | 0.3 |
| 59 | LYS | HN | -0.152 | 1 | 0.5 |
| 59 | LYS | HA | -0.142 | 1 | 0.3 |
| 60 | LYS | HN | -0.146 | 1 | 0.5 |
| 60 | LYS | HA | -0.139 | 1 | 0.3 |
| 61 | ASN | HA | -0.027 | 1 | 0.3 |
| 62 | VAL | HN | -0.201 | 1 | 0.5 |
| 62 | VAL | HA | -0.099 | 1 | 0.3 |
| 62 | VAL | HB | -0.085 | 1 | 0.3 |
| 63 | LEU | HN | -0.15 | 1 | 0.5 |
| 63 | LEU | HA | -0.16 | 1 | 0.3 |

| | | | | | |
|---|---|---|---|---|---|
| 63 | LEU | HG | -0.124 | 1 | 0.3 |
| 64 | TRP | HN | -0.064 | 1 | 0.5 |
| 64 | TRP | HA | -0.149 | 1 | 0.3 |
| 64 | TRP | HD1 | -0.117 | 1 | 0.3 |
| 64 | TRP | HE3 | -0.136 | 1 | 0.3 |
| 64 | TRP | HE1 | -0.111 | 1 | 0.3 |
| 64 | TRP | HZ3 | -0.138 | 1 | 0.3 |
| 64 | TRP | HZ2 | -0.082 | 1 | 0.3 |
| 65 | ASP | HN | 0.013 | 1 | 0.5 |
| 67 | ASN | HN | -0.661 | 1 | 0.5 |
| 67 | ASN | HA | -0.158 | 1 | 0.3 |
| 68 | ASN | HN | -0.19 | 1 | 0.5 |
| 68 | ASN | HA | -0.127 | 1 | 0.3 |
| 69 | MET | HN | -0.45 | 1 | 0.5 |
| 70 | SER | HN | -0.538 | 1 | 0.5 |
| 70 | SER | HA | -0.534 | 1 | 0.3 |
| 71 | GLU | HN | -0.136 | 1 | 0.5 |
| 71 | GLU | HA | -0.158 | 1 | 0.3 |
| 72 | TYR | HN | -0.126 | 1 | 0.5 |
| 72 | TYR | HA | -0.169 | 1 | 0.3 |
| 73 | LEU | HN | -0.155 | 1 | 0.5 |
| 73 | LEU | HA | -0.182 | 1 | 0.3 |
| 73 | LEU | HG | -1.057 | 1 | 0.3 |
| 74 | THR | HN | -0.138 | 1 | 0.5 |
| 74 | THR | HA | -0.137 | 1 | 0.3 |
| 74 | THR | HB | -0.132 | 1 | 0.3 |
| 74 | THR | HG21 | -0.022 | 3 | 0.3 |
| 74 | THR | HG22 | -0.022 | 3 | 0.3 |
| 74 | THR | HG23 | -0.022 | 3 | 0.3 |
| 75 | ASN | HN | -0.154 | 1 | 0.5 |
| 75 | ASN | HA | -0.2 | 1 | 0.3 |
| 80 | ILE | HN | -0.643 | 1 | 0.8 |
| 80 | ILE | HA | -0.259 | 1 | 0.8 |
| 80 | ILE | HB | 0.254 | 1 | 0.8 |
| 80 | ILE | HG21 | -1.345 | 3 | 0.8 |
| 80 | ILE | HG22 | -1.345 | 3 | 0.8 |
| 80 | ILE | HG23 | -1.345 | 3 | 0.8 |
| 80 | ILE | HG12 | -0.133 | 1 | 0.8 |
| 80 | ILE | HG13 | -0.133 | 1 | 0.8 |
| 86 | ALA | HA | -0.517 | 1 | 0.8 |
| 86 | ALA | HB1 | -0.722 | 3 | 0.8 |
| 86 | ALA | HB2 | -0.722 | 3 | 0.8 |
| 86 | ALA | HB3 | -0.722 | 3 | 0.8 |
| 87 | PHE | HZ | 0.273 | 1 | 0.8 |
| 87 | PHE | HD1 | 0.12 | 2 | 0.8 |
| 87 | PHE | HD2 | 0.12 | 2 | 0.8 |
| 87 | PHE | HE1 | -0.427 | 2 | 0.8 |
| 87 | PHE | HE2 | -0.427 | 2 | 0.8 |
| 89 | GLY | HN | -1.196 | 1 | 0.8 |
| 90 | LEU | HN | -0.66 | 1 | 0.8 |
| 90 | LEU | HA | -0.65 | 1 | 0.8 |
| 90 | LEU | HG | -0.764 | 1 | 0.8 |
| 91 | LYS | HN | -0.299 | 1 | 0.8 |

| | | | | | |
|---|---|---|---|---|---|
| 91 | LYS | HA | 0.206 | 1 | 0.8 |
| 92 | LYS | HN | -0.899 | 1 | 0.8 |
| 92 | LYS | HA | -0.882 | 1 | 0.8 |
| 95 | ASP | HN | -0.156 | 1 | 0.5 |
| 95 | ASP | HA | -0.136 | 1 | 0.3 |
| 95 | ASP | HB2 | -0.153 | 1 | 0.3 |
| 95 | ASP | HB3 | -0.151 | 1 | 0.3 |
| 96 | ARG | HN | -0.133 | 1 | 0.5 |
| 96 | ARG | HA | -0.154 | 1 | 0.3 |
| 97 | ASN | HN | -0.14 | 1 | 0.5 |
| 97 | ASN | HA | 0.585 | 1 | 0.3 |
| 98 | ASP | HN | -0.158 | 1 | 0.5 |
| 98 | ASP | HA | -0.144 | 1 | 0.3 |
| 99 | LEU | HN | -0.108 | 1 | 0.5 |
| 99 | LEU | HA | -0.139 | 1 | 0.3 |
| 100 | ILE | HN | -0.105 | 1 | 0.5 |
| 100 | ILE | HA | -0.126 | 1 | 0.3 |
| 100 | ILE | HB | -0.154 | 1 | 0.3 |
| 100 | ILE | HG21 | -0.57 | 3 | 0.3 |
| 100 | ILE | HG22 | -0.57 | 3 | 0.3 |
| 100 | ILE | HG23 | -0.57 | 3 | 0.3 |
| 100 | ILE | HG12 | -1 | 1 | 0.3 |
| 100 | ILE | HG13 | -1 | 1 | 0.3 |
| 100 | ILE | HD11 | -0.583 | 3 | 0.3 |
| 100 | ILE | HD12 | -0.583 | 3 | 0.3 |
| 100 | ILE | HD13 | -0.583 | 3 | 0.3 |
| 101 | THR | HN | -0.163 | 1 | 0.5 |
| 101 | THR | HA | -0.752 | 1 | 0.3 |
| 101 | THR | HG21 | -0.127 | 3 | 0.3 |
| 101 | THR | HG22 | -0.127 | 3 | 0.3 |
| 101 | THR | HG23 | -0.127 | 3 | 0.3 |
| 102 | TYR | HN | -0.225 | 1 | 0.5 |
| 102 | TYR | HA | -0.127 | 1 | 0.3 |
| 103 | LEU | HN | -0.07 | 1 | 0.5 |
| 103 | LEU | HA | -0.091 | 1 | 0.3 |
| 104 | LYS | HN | -0.223 | 1 | 0.5 |
| 104 | LYS | HA | -0.216 | 1 | 0.3 |
| 105 | LYS | HN | -0.209 | 1 | 0.5 |
| 105 | LYS | HA | -0.141 | 1 | 0.3 |
| 106 | ALA | HN | -0.119 | 1 | 0.5 |
| 106 | ALA | HA | -0.145 | 1 | 0.3 |
| 106 | ALA | HB1 | -0.132 | 3 | 0.3 |
| 106 | ALA | HB2 | -0.132 | 3 | 0.3 |
| 106 | ALA | HB3 | -0.132 | 3 | 0.3 |
| 107 | THR | HN | -0.461 | 1 | 0.5 |
| 107 | THR | HA | -0.009 | 1 | 0.3 |
| 107 | THR | HG21 | -0.127 | 3 | 0.3 |
| 107 | THR | HG22 | -0.127 | 3 | 0.3 |
| 107 | THR | HG23 | -0.127 | 3 | 0.3 |
| 108 | GLU | HN | -0.229 | 1 | 0.5 |
| 108 | GLU | HA | -0.133 | 1 | 0.3 |

**Table III**. Experimental NOESY cross peak intensities (last column) and corresponding upper distance limits (3rd column, Å). The nomenclature of the atoms is that used by the program DYANA (J Mol Biol. 1997 Oct 17;273(1):283-98). The heme is called HEC 18, and this residue includes atoms from both the heme and the proximal ligand histine. The reported volumes of cross-peaks involving pseudoatoms correspond to the measured volumes divided by the number of atoms represented by the pseudoatom (a symbol *2 or *4 is present in these cases).

| Atom 1 | | Atom 2 | | upl | volume |
|---|---|---|---|---|---|
| -3 PHE | | | | | |
| | HN | -3 PHE | QB | 4.4 | 40340 *2 |
| | HN | -2 LYS | HN | 4.3 | 23790 |
| | HA | -3 PHE | QB | 4.6 | 55950 *2 |
| 14 LEU | | | | | |
| | HN | 9 LEU | HA | 4.3 | 21320 |
| | HN | 9 LEU | HB2 | 4 | 33540 |
| | HN | 9 LEU | HB3 | 4.1 | 30150 |
| | HN | 9 LEU | HG | 4.2 | 48250 |
| | HN | 9 LEU | QD1 | 5.7 | 16080 |
| | HN | 9 LEU | QD2 | 5.7 | 16779 |
| | HN | 10 PHE | HN | 4.6 | 16389 |
| | HN | 10 PHE | QB | 6.5 | 345.8 *2 |
| | HN | 11 LYS | HN | 5.2 | 8000 |
| | HA | 9 LEU | HB3 | 5.5 | 2958 |
| | HA | 9 LEU | QD1 | 3.9 | 104800 |
| | HA | 10 PHE | HN | 5.5 | 3729 |
| | HA | 11 LYS | HN | 5.5 | 584 |
| | HA | 11 LYS | HG2 | 5.5 | 3266 |
| | HA | 12 THR | HN | 5.4 | 6873 |
| | HB2 | 9 LEU | QD1 | 3.6 | 165400 |
| | HB2 | 10 PHE | HN | 5.5 | 2810.1 |
| | HB2 | 94 LEU | HN | 5.5 | 1236 |
| | HB3 | 9 LEU | HG | 3.2 | 199000 |
| | HB3 | 9 LEU | QD1 | 5.4 | 21620 |
| | HB3 | 10 PHE | HN | 4.3 | 21750 |
| | HB3 | 13 ARG | QG | 4.8 | 46955 *2 |
| | HB3 | 94 LEU | QD2 | 3.3 | 163900 |
| | HG | 10 PHE | HN | 5.5 | 12660 |
| | HG | 13 ARG | QG | 6.5 | 9325 *2 |
| | HG | 90 ASP | HA | 5.5 | 10370 |
| | HG | 90 ASP | HB2 | 4.4 | 35990 |
| | HG | 93 ASP | QB | 5.4 | 35950 *2 |
| | QD1 | 10 PHE | HN | 6.5 | 1927 |
| | QD1 | 90 ASP | HA | 6.5 | 5900 |
| | QD1 | 91 ARG | HA | 5 | 72700 |
| | QD1 | 94 LEU | HN | 6.5 | 1980 |
| | QD1 | 94 LEU | QD2 | 4.3 | 166000 |
| | QD2 | 10 PHE | HN | 6.5 | 2777.1 |
| 10 PHE | | | | | |
| | HN | 10 PHE | HA | 4 | 30810 |
| | HN | 10 PHE | QB | 4.1 | 60100 *2 |
| | HN | 10 PHE | CG | 7.5 | 7563 *2 |
| | HN | 11 LYS | HN | 4.6 | 15850 |
| | HN | 11 LYS | QB | 6.5 | 1386 *2 |
| | HN | 90 ASP | HB3 | 5.5 | 2860 |
| | HN | 94 LEU | HB2 | 5.5 | 1444.2 |
| | HN | 94 LEU | QD2 | 6.5 | 34950 |
| | HA | 10 PHE | QB | 6.5 | 1242 *2 |
| | HA | 10 PHE | CG | 5.8 | 25460 *2 |
| | HA | 11 LYS | HN | 3.8 | 40410 |
| | HA | 13 ARG | HN | 5 | 11180 |
| | HA | 14 CYS | HN | 4.3 | 26960 |
| | HA | 14 CYS | HB2 | 4.9 | 11930 |
| | HA | 14 CYS | HB3 | 3.7 | 70280 |
| | HA | 15 LEU | HN | 4.9 | 6354 |
| | HA | 94 LEU | QD2 | 3.3 | 185800 |
| | QB | 10 PHE | CG | 7.4 | 38700 *4 |
| | QB | 11 LYS | HN | 5.7 | 14136 *2 |
| | QB | 94 LEU | QD2 | 7.5 | 28380 *2 |
| | QB | 97 TYR | HB2 | 4.6 | 50900 *2 |
| | CG | 10 PHE | HZ | 7.5 | 321 *2 |
| | CG | 11 LYS | HN | 7.5 | 8524.5 *2 |
| | CG | 11 LYS | QB | 8.5 | 1897.2 *4 |
| | CG | 14 CYS | HN | 7.5 | 274.5 *2 |
| | CG | 14 CYS | HB2 | 7.5 | 15335 *2 |
| | CG | 14 CYS | HB3 | 7.3 | 26175 *2 |
| | CG | 15 LEU | HN | 7.5 | 21055 *2 |
| | CG | 15 LEU | QD1 | 8.5 | 31305 *2 |
| | CG | 15 LEU | QD2 | 8.5 | 11395 *2 |
| | CG | 18 HEC | HB2 | 7.5 | 279 *2 |
| | CG | 19 THR | HA | 7.5 | 9710 *2 |
| | CG | 94 LEU | QD2 | 7.6 | 60200 *2 |
| | CG | 98 LEU | HG | 7.5 | 3298 *2 |
| | CG | 98 LEU | QD1 | 8.5 | 15400 *2 |
| | HZ | 18 HEC | HN | 5.5 | 2432 |
| | HZ | 18 HEC | HA | 5.5 | 951 |
| | HZ | 18 HEC | HB2 | 5.2 | 27110 |
| | HZ | 18 HEC | HB3 | 5.5 | 16370 |
| | HZ | 32 LEU | QD2 | 5.5 | 62240 |
| 11 LYS | | | | | |
| | HN | 11 LYS | HA | 3.7 | 47460 |
| | HN | 11 LYS | QB | 4.2 | 56450 *2 |
| | HN | 11 LYS | HG2 | 3.9 | 69930 |

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| | HN | 11 LYS | HG3 | 4.2 | 49500 | | HN | 15 LEU | HN | 3.3 | 87790 |
| | HN | 11 LYS | HD2 | 4.3 | 47610 | | HN | 15 LEU | HA | 4.5 | 18765 |
| | HN | 11 LYS | HD3 | 5 | 21396 | | HN | 15 LEU | QD2 | 6.5 | 14420 |
| | HN | 12 THR | HN | 3.5 | 66480 | | HA | 14 CYS | HB2 | 3.7 | 47140 |
| | HN | 12 THR | QG2 | 6.5 | 9859 | | HA | 14 CYS | HB3 | 5 | 10900 |
| | HA | 11 LYS | HG2 | 5 | 21950 | | HA | 15 LEU | HN | 5.5 | 2725 |
| | HA | 11 LYS | HG3 | 4.2 | 51210 | | HB3 | 15 LEU | HN | 4.1 | 29865 |
| | HA | 11 LYS | HD2 | 5.5 | 5989 | 15 LEU | | | | | |
| | QB | 11 LYS | HD3 | 4.8 | 79750 *2 | | HN | 15 LEU | HA | 3.6 | 58140 |
| | QB | 12 THR | HN | 5.5 | 17205 *2 | | HN | 15 LEU | QD1 | 5.2 | 74780 |
| | QB | 15 LEU | QD2 | 4.8 | 118000 *2 | | HN | 15 LEU | QD2 | 4.2 | 73590 |
| | HG2 | 12 THR | HN | 5.5 | 2907 | | HA | 15 LEU | QD1 | 6.5 | 7375 |
| | HG3 | 12 THR | HN | 5.5 | 16330 | | HA | 15 LEU | QD2 | 3.3 | 294500 |
| | HD3 | 12 THR | QG2 | 6.5 | 22860 | | HA | 17 CYS | HN | 5.5 | 2192 |
| 12 THR | | | | | | | HA | 19 THR | HA | 5.5 | 3007 |
| | HN | 12 THR | HA | 3.9 | 39210 | 16 GLN | | | | | |
| | HN | 12 THR | HB | 5.1 | 9621 | | HN | 16 GLN | HA | 4.7 | 14820 |
| | HN | 12 THR | QG2 | 4.9 | 36130 | | HN | 16 GLN | HB2 | 4.2 | 25005 |
| | HN | 13 ARG | HN | 4.1 | 28023 | | HN | 16 GLN | HB3 | 4.1 | 28635 |
| | HN | 16 GLN | HE21 | 5.3 | 25866 | | HN | 16 GLN | HE22 | 5.5 | 3789 |
| | HA | 12 THR | QG2 | 3.4 | 236300 | | HA | 16 GLN | HE21 | 4.8 | 26310 |
| | HA | 13 ARG | HN | 4.6 | 15423 | | HA | 16 GLN | HE22 | 5.5 | 9852 |
| | HA | 16 GLN | HE21 | 5.5 | 1982.7 | | HB2 | 16 GLN | HE21 | 5.1 | 19923 |
| | HA | 16 GLN | HE22 | 5.5 | 2167.8 | | HB2 | 16 GLN | HE22 | 5.5 | 10431 |
| | HB | 13 ARG | HN | 5.5 | 6411 | | HB3 | 16 GLN | HE21 | 5.5 | 6210 |
| | QG2 | 13 ARG | HN | 6.5 | 19670 | | HG2 | 16 GLN | HE21 | 5.5 | 4623 |
| 13 ARG | | | | | | | HG2 | 16 GLN | HE22 | 5.5 | 5190 |
| | HN | 13 ARG | HA | 4.1 | 27969 | | HG3 | 16 GLN | HE22 | 5.5 | 4449 |
| | HN | 13 ARG | HB2 | 4 | 33450 | | HE22 | 18 HEC | HB2 | 5.5 | 2133 |
| | HN | 13 ARG | HB3 | 4.2 | 24315 | | HE22 | 18 HEC | QM3 | 6.5 | 3565 |
| | HN | 13 ARG | QG | 6.1 | 19300 *2 | 17 CYS | | | | | |
| | HN | 14 CYS | HN | 3.1 | 110670 | | HN | 17 CYS | HA | 5.5 | 2098 |
| | HN | 14 CYS | HA | 5.5 | 4269 | | HN | 17 CYS | QB | 6.1 | 1812 *2 |
| | HN | 14 CYS | HB3 | 5.5 | 6219 | | HN | 18 HEC | HN | 4.3 | 21600 |
| | HN | 15 LEU | HN | 5.2 | 8262 | | QB | 18 HEC | HN | 6.5 | 539.7 *2 |
| | HA | 13 ARG | HB2 | 4.6 | 16230 | 18 HEC | | | | | |
| | HA | 13 ARG | HB3 | 4.6 | 15470 | | HN | 18 HEC | HD2 | 5 | |
| | HA | 13 ARG | QG | 6.1 | 6365 *2 | | HA | 30 PRO | HA | 5 | |
| | HA | 14 CYS | HN | 5.1 | 9375 | | HB2 | 18 HEC | HD2 | 5 | |
| | HB2 | 13 ARG | QG | 4.6 | 104800 *2 | | HB3 | 18 HEC | HD1 | 5 | |
| | HB2 | 14 CYS | HN | 5.5 | 972 | | HD1 | 18 HEC | HE1 | 5 | |
| | HB3 | 13 ARG | QG | 5 | 63900 *2 | | QM8 | 59 TRP | HE1 | 5 | |
| | HB3 | 14 CYS | HN | 4.4 | 21231 | | HN | 18 HEC | HA | 4 | 31730 |
| | HB3 | 15 LEU | HN | 5.5 | 2448.3 | | HN | 18 HEC | HB2 | 4.5 | 17450 |
| | QG | 14 CYS | HN | 6.5 | 9789 *2 | | HN | 18 HEC | HB3 | 4.6 | 16910 |
| | QG | 82 PHE | HZ | 5.3 | 37000 *2 | | HN | 18 HEC | QM3 | 6.1 | 11280 |
| | QG | 90 ASP | HA | 6.5 | 3430.5 *2 | | HN | 19 THR | HN | 5.5 | 3826 |
| | QG | 94 LEU | HB3 | 6.5 | 13370 *2 | | HA | 18 HEC | HB2 | 4.5 | 18170 |
| | QG | 94 LEU | QD2 | 7.5 | 1387 *2 | | HA | 18 HEC | HB3 | 4 | 32260 |
| 14 CYS | | | | | | | HA | 19 THR | HN | 3.2 | 100500 |
| | HN | 14 CYS | HA | 4.2 | 24960 | | HA | 19 THR | HA | 5.5 | 1947 |
| | HN | 14 CYS | HB2 | 4.1 | 30010 | | HA | 19 THR | QG2 | 6.5 | 14600 |
| | HN | 14 CYS | HB3 | 4.1 | 29637 | | HA | 30 PRO | HA | 5.5 | 674 |

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| | HA | 31 ASN | HA | 4.8 | 6653 | 20 VAL | | | | | |
| | HA | 32 LEU | QD2 | 6.5 | 2291 | | HN | 20 VAL | HA | 5.5 | 2781 |
| | HB2 | 19 THR | HN | 5.5 | 3409 | | HA | 31 ASN | HA | 5.3 | 3558 |
| | HB2 | 32 LEU | QD2 | 6.5 | 2306 | | HA | 31 ASN | HD21 | 5.5 | 2177.7 |
| | HB3 | 19 THR | HN | 5.4 | 6965 | | HA | 32 LEU | HN | 3.9 | 24432 |
| | HB3 | 19 THR | HA | 5.5 | 4173 | | HA | 33 HIS | HN | 5.1 | 4497 |
| | HB3 | 29 GLY | HN | 5.5 | 1185 | 24 GLY | | | | | |
| | HB3 | 32 LEU | HB3 | 5.5 | 1813 | | HA1 | 31 ASN | HD21 | 5.5 | 12912 |
| | HB3 | 32 LEU | QD2 | 6.5 | 17890 | 29 GLY | | | | | |
| | HD1 | 32 LEU | QD2 | 6.5 | 1348 | | HN | 29 GLY | HA1 | 5.4 | 7299 |
| | QM8 | 18 HEC | HDM | 6.1 | 11300 | | HN | 29 GLY | HA2 | 3.9 | 37030 |
| | QM8 | 32 LEU | QD2 | 6.5 | 14250 | | HN | 30 PRO | HA | 5.5 | 2960 |
| | QM8 | 64 MET | QE | 6.5 | 2461 | | HA1 | 30 PRO | HA | 4.8 | 12320 |
| | HDM | 18 HEC | QM1 | 5.5 | 19060 | | HA1 | 30 PRO | HD2 | 3.9 | 44300 |
| | QM1 | 18 HEC | HT2A | 4.4 | 58020 | | HA1 | 30 PRO | HD3 | 3 | 76540 |
| | QM1 | 18 HEC | QT2 | 5.2 | 27030 | | HA2 | 30 PRO | HA | 5.1 | 9696 |
| | QM1 | 32 LEU | QD2 | 6.5 | 4697 | | HA2 | 30 PRO | HD2 | 3.3 | 60680 |
| | HT2A | 18 HEC | QT2 | 3.5 | 178500 | | HA2 | 48 TYR | CZ | 7.5 | 656.5 *2 |
| | HT2A | 71 PRO | HA | 3.8 | 45330 | 30 PRO | | | | | |
| | HT2A | 72 ALA | HN | 5.4 | 25670 | | HA | 30 PRO | HD2 | 5 | |
| | HT2A | 73 LYS | HN | 5.5 | 3064 | | HA | 30 PRO | HG2 | 4.7 | 27850 |
| | HT2A | 73 LYS | HB2 | 5.5 | 262 | | HA | 30 PRO | HG3 | 5.5 | 1801 |
| | HT2A | 73 LYS | HG2 | 5.5 | 5874 | | HA | 30 PRO | HD3 | 5.5 | 780 |
| | HT2A | 82 PHE | CG | 7.5 | 6220 *2 | | HA | 32 LEU | QD2 | 6.5 | 288 |
| | HT2A | 82 PHE | CZ | 7.5 | 16130 *2 | | HG2 | 30 PRO | HD3 | 5.5 | 2754 |
| | HT2A | 82 PHE | HZ | 4.8 | 30410 | | HG2 | 46 TYR | HN | 5.5 | 7105 |
| | QT2 | 72 ALA | HN | 6.5 | 13480 | | HG3 | 30 PRO | HD2 | 4.5 | 34440 |
| | QT2 | 82 PHE | CG | 8.5 | 4832.5 *2 | | HG3 | 30 PRO | HD3 | 3.4 | 139700 |
| | QT2 | 82 PHE | CZ | 8.5 | 8985 *2 | | HG3 | 46 TYR | HN | 5.5 | 4502 |
| | QT2 | 82 PHE | HZ | 6.5 | 3486 | | HG3 | 48 TYR | CZ | 7.5 | 983.5 *2 |
| | QM5 | 29 GLY | HA1 | 6.3 | 50840 | | HD3 | 46 TYR | HN | 5.5 | 1876 |
| | QM5 | 29 GLY | HA2 | 6.5 | 27230 | 31 ASN | | | | | |
| | QM5 | 30 PRO | HG3 | 6.5 | 5177 | | HA | 31 ASN | HD21 | 5.5 | 5752 |
| | QM5 | 30 PRO | HD2 | 6.5 | 19990 | | HA | 31 ASN | HD22 | 5.5 | 7349 |
| | QM5 | 30 PRO | HD3 | 6.5 | 12390 | | HA | 32 LEU | HN | 3.3 | 91350 |
| 19 THR | | | | | | | HA | 32 LEU | HB2 | 5.5 | 2671 |
| | HN | 19 THR | HA | 4.8 | 12640 | | HA | 33 HIS | HN | 4.9 | 12354 |
| | HN | 19 THR | HB | 5.5 | 1491.6 | | HD21 | 32 LEU | HN | 5.5 | 2280.6 |
| | HN | 19 THR | QG2 | 4.9 | 34890 | 32 LEU | | | | | |
| | HN | 31 ASN | HA | 3.9 | 24850 | | HN | 32 LEU | HA | 4.7 | 14670 |
| | HN | 32 LEU | HN | 5.5 | 3095 | | HN | 32 LEU | HB2 | 4 | 33210 |
| | HA | 19 THR | HB | 3.2 | 105100 | | HN | 32 LEU | HB3 | 4.6 | 16340 |
| | HA | 19 THR | QG2 | 4 | 99030 | | HN | 32 LEU | QD1 | 6.5 | 1980 |
| | HA | 20 VAL | HN | 5.5 | 2957 | | HN | 32 LEU | QD2 | 5.5 | 19368 |
| | HA | 20 VAL | HA | 5.5 | 1738 | | HN | 33 HIS | HN | 3.7 | 47340 |
| | HB | 19 THR | QG2 | 4 | 97170 | | HA | 32 LEU | HB3 | 5.5 | 2293 |
| | HB | 21 GLU | HN | 5.5 | 3783 | | HA | 32 LEU | QD1 | 6 | 12090 |
| | HB | 31 ASN | HD21 | 5.5 | 1559.1 | | HA | 32 LEU | QD2 | 6.5 | 143 |
| | QG2 | 20 VAL | HN | 6.5 | 3708 | | HA | 33 HIS | HN | 4.9 | 11124 |
| | QG2 | 30 PRO | HA | 6.5 | 669 | | HA | 33 HIS | HA | 5.5 | 564 |
| | QG2 | 31 ASN | HD21 | 6.5 | 5289 | | HB2 | 32 LEU | QD1 | 6.5 | 3297 |
| | QG2 | 31 ASN | HD22 | 6.5 | 3782 | | HB2 | 33 HIS | HN | 4.4 | 19980 |
| | QG2 | 32 LEU | HN | 6.5 | 2175 | | HB2 | 33 HIS | HA | 5.5 | 6503 |

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| | HB3 | 32 LEU | QD1 | 3.3 | 275600 |
| | HB3 | 33 HIS | HN | 3.6 | 55080 |
| | QD2 | 33 HIS | HN | 6.5 | 12411 |
| 33 HIS | | | | | |
| | HN | 33 HIS | HA | 4 | 33810 |
| | HN | 33 HIS | HB2 | 3.4 | 74790 |
| | HN | 33 HIS | HB3 | 3.4 | 73590 |
| | HA | 33 HIS | HB3 | 5.5 | 4775 |
| | HA | 34 GLY | HA2 | 5.4 | 7459 |
| | HA | 98 LEU | QD1 | 6.5 | 4266 |
| | HA | 102 THR | QG2 | 6.5 | 1854 |
| 34 GLY | | | | | |
| | HA1 | 35 ILE | HN | 4.3 | 21880 |
| | HA2 | 35 ILE | HN | 3.9 | 38990 |
| | HA2 | 36 PHE | HN | 5.1 | 9901 |
| | HA2 | 36 PHE | CG | 7.5 | 6425 *2 |
| | HA2 | 36 PHE | HZ | 5.5 | 5233 |
| | HA2 | 98 LEU | HA | 5.2 | 4287 |
| | HA2 | 98 LEU | QD2 | 6.5 | 648 |
| 35 ILE | | | | | |
| | HN | 35 ILE | HA | 3.4 | 76320 |
| | HN | 35 ILE | HB | 3.2 | 97460 |
| | HN | 35 ILE | QG2 | 6.5 | 2657.7 |
| | HN | 35 ILE | HG12 | 5.4 | 14890 |
| | HN | 35 ILE | HG13 | 5.5 | 8457 |
| | HN | 35 ILE | QD1 | 4.6 | 46290 |
| | HN | 36 PHE | HN | 4.2 | 26421 |
| | HN | 36 PHE | CZ | 7.5 | 3388 *2 |
| | HN | 98 LEU | QD1 | 6.5 | 13070 |
| | HN | 98 LEU | QD2 | 6.5 | 1108 |
| | HA | 35 ILE | HB | 4.2 | 24550 |
| | HA | 35 ILE | HG12 | 4.1 | 54100 |
| | HA | 35 ILE | HG13 | 5.1 | 19880 |
| | HA | 35 ILE | QD1 | 5.2 | 26180 |
| | HA | 36 PHE | HN | 4.1 | 27180 |
| | HA | 38 ARG | HB3 | 5.5 | 516 |
| | HA | 38 ARG | QG | 6.5 | 98 *2 |
| | HA | 38 ARG | QD | 6.5 | 1093.5 *2 |
| | HB | 35 ILE | HG12 | 3.9 | 74640 |
| | HB | 35 ILE | QD1 | 3.9 | 106400 |
| | HB | 36 PHE | HN | 5.5 | 3973 |
| | HB | 95 ILE | QD1 | 4.9 | 73580 |
| | HB | 98 LEU | QD1 | 4.4 | 90000 |
| | QG2 | 35 ILE | QD1 | 4.6 | 169100 |
| | QG2 | 36 PHE | HN | 6.5 | 711 |
| | QG2 | 36 PHE | HZ | 6.5 | 1232 |
| | QG2 | 64 MET | QE | 7.5 | 396 |
| | QG2 | 95 ILE | QG1 | 7.5 | 2862.5 *2 |
| | QG2 | 98 LEU | QD1 | 5.5 | 86830 |
| | HG12 | 35 ILE | QD1 | 4.8 | 40450 |
| | HG12 | 38 ARG | HB3 | 3 | 74720 |
| | HG12 | 59 TRP | HD1 | 5.5 | 20480 |
| | HG13 | 35 ILE | QD1 | 4.8 | 38320 |
| | HG13 | 59 TRP | HB3 | 5.5 | 8176 |
| | HG13 | 59 TRP | HD1 | 5.5 | 1992 |
| | HG13 | 59 TRP | HE3 | 5.5 | 5670 |
| | HG13 | 68 LEU | QD1 | 6.5 | 6410 |
| | HG13 | 94 LEU | QD2 | 6.5 | 1769 |
| | QD1 | 36 PHE | HN | 6.5 | 34570 |
| | QD1 | 36 PHE | CG | 8.5 | 19545 *2 |
| | QD1 | 36 PHE | CZ | 8.5 | 9420 *2 |
| | QD1 | 59 TRP | HB3 | 6.5 | 1306 |
| | QD1 | 68 LEU | QD1 | 4.3 | 234900 |
| | QD1 | 94 LEU | HG | 5.9 | 56270 |
| | QD1 | 94 LEU | QD2 | 4.5 | 132400 |
| | QD1 | 95 ILE | QG1 | 7.5 | 1056 *2 |
| | QD1 | 95 ILE | QD1 | 5.8 | 77110 |
| | QD1 | 98 LEU | QD1 | 7.5 | 12020 |
| 36 PHE | | | | | |
| | HN | 36 PHE | HA | 4.5 | 17760 |
| | HN | 36 PHE | QB | 4.5 | 35580 *2 |
| | HN | 36 PHE | CG | 6.6 | 31125 *2 |
| | HN | 36 PHE | CZ | 6.5 | 1715 *2 |
| | HN | 37 GLY | HN | 4.6 | 16005 |
| | HN | 38 ARG | HN | 3.8 | 57470 |
| | HN | 64 MET | QE | 6.5 | 889 |
| | HN | 99 LYS | QD | 6.5 | 11500 *2 |
| | HN | 103 GLU | QG | 6.5 | 3229.5 *2 |
| | HA | 36 PHE | CG | 6.5 | 10225 *2 |
| | HA | 37 GLY | HN | 5.5 | 2460 |
| | HA | 59 TRP | HB2 | 5.5 | 1997 |
| | QB | 36 PHE | CG | 7.7 | 29225 *4 |
| | QB | 36 PHE | CZ | 8.5 | 1590 *4 |
| | QB | 37 GLY | HN | 5.7 | 15030 *2 |
| | CG | 36 PHE | CZ | 8.5 | 35175 *4 |
| | CG | 37 GLY | HN | 7.5 | 5580 *2 |
| | CG | 95 ILE | QG1 | 8.5 | 2810 *4 |
| | CG | 95 ILE | QD1 | 8.5 | 1902.5 *2 |
| | CG | 99 LYS | HA | 7.1 | 28240 *2 |
| | CG | 99 LYS | QG | 8.5 | 2114.5 *4 |
| | CG | 99 LYS | QD | 8.5 | 2530 *4 |
| | CZ | 36 PHE | HZ | 6.3 | 43730 *2 |
| | CZ | 64 MET | QE | 8.5 | 1700 *2 |
| | CZ | 95 ILE | QG1 | 8.5 | 1391.8 *4 |
| | CZ | 95 ILE | QD1 | 8.5 | 13875 *2 |
| | CZ | 98 LEU | HN | 7.5 | 1507.5 *2 |
| | CZ | 98 LEU | HA | 7.5 | 1049 *2 |
| | CZ | 98 LEU | HB2 | 7.5 | 6580 *2 |
| | CZ | 98 LEU | HG | 7.5 | 19715 *2 |
| | CZ | 98 LEU | QD1 | 8.5 | 10430 *2 |
| | CZ | 98 LEU | QD2 | 8.5 | 168 *2 |
| | CZ | 99 LYS | HN | 7.5 | 1603 *2 |
| | CZ | 99 LYS | HA | 7.5 | 11655 *2 |
| | CZ | 99 LYS | QB | 8.5 | 170.8 *4 |
| | CZ | 99 LYS | QG | 8.5 | 1466 *4 |
| | CZ | 99 LYS | QD | 8.5 | 9380 *4 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | CZ | 103 GLU | HA | 7.5 | 989.5 *2 | | HN | 59 TRP | HD1 | 5.5 | 2209 |
| | CZ | 103 GLU | HB2 | 7.5 | 3376 *2 | | HA | 39 HIS | HB2 | 4.2 | 25000 |
| | HZ | 95 ILE | HA | 5.5 | 7893 | | HA | 39 HIS | HB3 | 4.2 | 26040 |
| | HZ | 95 ILE | QG1 | 6.5 | 4309 *2 | | HA | 39 HIS | HD1 | 5.5 | 1835 |
| | HZ | 95 ILE | QD1 | 6.5 | 27240 | | HA | 40 SER | HN | 3.5 | 59760 |
| | HZ | 98 LEU | HN | 5.5 | 1912 | | HA | 58 LEU | HA | 3.4 | 53070 |
| | HZ | 98 LEU | HB2 | 5.5 | 8345 | | HA | 58 LEU | QD1 | 6.5 | 13670 |
| | HZ | 98 LEU | QD1 | 6.5 | 16920 | | HA | 59 TRP | HN | 4.2 | 15663 |
| | HZ | 99 LYS | HN | 5.5 | 826 | | HA | 59 TRP | HE1 | 5.5 | 968 |
| | HZ | 99 LYS | HA | 5.5 | 2760 | | HB2 | 39 HIS | HD1 | 5.5 | 7057 |
| | HZ | 99 LYS | QB | 6.5 | 7625 *2 | | HB2 | 40 SER | HN | 4.3 | 21870 |
| | HZ | 99 LYS | QD | 6.5 | 12420 *2 | | HB3 | 39 HIS | HD1 | 5.1 | 19420 |
| 37 GLY | | | | | | | HB3 | 40 SER | HN | 3.7 | 45680 |
| | HN | 37 GLY | HA1 | 3 | 134670 | | HB3 | 57 VAL | HN | 5.5 | 4646 |
| | HN | 37 GLY | HA2 | 3.4 | 71880 | | HB3 | 59 TRP | HD1 | 5.5 | 12100 |
| | HN | 38 ARG | HN | 3.8 | 40580 | | HD1 | 40 SER | HN | 5.5 | 1209 |
| | HN | 59 TRP | HN | 5.5 | 1194.9 | | HD1 | 58 LEU | HN | 5.5 | 1828 |
| | HN | 59 TRP | HB2 | 5.5 | 4759 | | HD1 | 58 LEU | HA | 5.5 | 6941 |
| | HA1 | 38 ARG | HN | 4.1 | 28977 | | HD1 | 58 LEU | HB2 | 5.5 | 10500 |
| | HA1 | 59 TRP | HN | 3.9 | 22450 | | HD1 | 58 LEU | HB3 | 5.5 | 1013 |
| | HA2 | 38 ARG | HN | 3.9 | 35040 | | HD1 | 58 LEU | QD1 | 6.5 | 7231 |
| 38 ARG | | | | | | | HD1 | 58 LEU | QD2 | 6.5 | 2235 |
| | HN | 38 ARG | HA | 5.5 | 2535.9 | 40 SER | | | | | |
| | HN | 38 ARG | HB2 | 5.1 | 9924 | | HN | 40 SER | HA | 4.6 | 15660 |
| | HN | 38 ARG | HB3 | 4.7 | 14958 | | HN | 40 SER | HB3 | 5.4 | 7257 |
| | HN | 38 ARG | QG | 6.5 | 7250 *2 | | HN | 41 GLY | HN | 5.2 | 8589 |
| | HN | 38 ARG | QD | 6.5 | 11390 *2 | | HN | 56 ASN | HN | 5.5 | 1759.2 |
| | HN | 39 HIS | HN | 5.2 | 8862 | | HN | 57 VAL | HN | 4.2 | 15380 |
| | HN | 58 LEU | QD1 | 6.5 | 10476 | | HN | 57 VAL | HA | 4.7 | 33340 |
| | HN | 58 LEU | QD2 | 6.5 | 646 | | HN | 57 VAL | HB | 5.5 | 3362 |
| | HN | 59 TRP | HD1 | 5.5 | 4548 | | HN | 57 VAL | QG1 | 6.5 | 1211 |
| | HA | 39 HIS | HN | 5.5 | 3059 | | HN | 57 VAL | QG2 | 6.5 | 12910 |
| | HB2 | 39 HIS | HN | 5.3 | 7570 | | HN | 58 LEU | HA | 5.5 | 1425 |
| | HB2 | 42 GLN | HN | 4.8 | 13368 | | HN | 59 TRP | HN | 5.5 | 540 |
| | HB2 | 59 TRP | HD1 | 5.5 | 1960 | | HN | 59 TRP | HD1 | 5.5 | 2803 |
| | HB2 | 59 TRP | HE1 | 5.5 | 20520 | | HN | 59 TRP | HE1 | 3.9 | 43030 |
| | HB3 | 39 HIS | HN | 3.8 | 43920 | | HA | 41 GLY | HN | 3.4 | 78550 |
| | HB3 | 59 TRP | HD1 | 5.5 | 1812 | | HA | 41 GLY | HA2 | 5.5 | 824 |
| | QG | 39 HIS | HN | 6.5 | 5419.5 *2 | | HA | 52 ASN | HD21 | 5.5 | 6658 |
| | QG | 59 TRP | HB2 | 6.5 | 360 *2 | | HA | 57 VAL | QG2 | 6.5 | 6809 |
| | QG | 59 TRP | HB3 | 6.5 | 4804 *2 | | HA | 59 TRP | HD1 | 5.5 | 8075 |
| | QG | 59 TRP | HD1 | 6.5 | 2005.5 *2 | | HA | 59 TRP | HE1 | 5.5 | 11930 |
| | QG | 59 TRP | HE1 | 6.5 | 707 *2 | | HA | 59 TRP | HZ2 | 5.5 | 3637 |
| | QD | 39 HIS | HN | 6.5 | 7290 *2 | | HB2 | 57 VAL | HN | 3.4 | 55980 |
| | QD | 59 TRP | HD1 | 6.5 | 8120 *2 | | HB3 | 57 VAL | HN | 5.5 | 971 |
| 39 HIS | | | | | | | HB3 | 57 VAL | HB | 5.5 | 13010 |
| | HN | 39 HIS | HA | 5.5 | 5991 | | HB3 | 57 VAL | QG2 | 6.5 | 2113 |
| | HN | 39 HIS | HB2 | 3.7 | 45790 | 41 GLY | | | | | |
| | HN | 39 HIS | HB3 | 4.3 | 22790 | | HN | 41 GLY | HA1 | 3.8 | 41640 |
| | HN | 39 HIS | HD1 | 5.5 | 335.7 | | HN | 41 GLY | HA2 | 4 | 32380 |
| | HN | 40 SER | HN | 5.5 | 1743 | | HN | 48 TYR | CZ | 7.5 | 217.5 *2 |
| | HN | 58 LEU | HA | 5.5 | 1369 | | HN | 52 ASN | HD21 | 5.5 | 4048 |
| | HN | 58 LEU | QD1 | 6.5 | 5041 | | HN | 57 VAL | QG2 | 6.5 | 258 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | HN | 59 TRP | HE1 | 5.5 | 4751 | | HB2 | 48 TYR | CG | 7.5 | 12725 *2 |
| | HA1 | 43 ALA | HN | 5.5 | 1218 | | HB2 | 48 TYR | CZ | 7.5 | 2058 *2 |
| | HA1 | 48 TYR | CG | 7.5 | 2319.5 *2 | | HB2 | 53 ILE | QG2 | 3.3 | 166400 |
| | HA1 | 48 TYR | CZ | 7.5 | 1314.5 *2 | | CG | 48 TYR | CZ | 8.3 | 47675 *4 |
| | HA2 | 43 ALA | HN | 5.5 | 315 | 49 THR | | | | | |
| | HA2 | 48 TYR | CZ | 7.5 | 3037 *2 | | HN | 49 THR | QG2 | 4.7 | 41850 |
| | HA2 | 52 ASN | HD22 | 5.5 | 513 | 52 ASN | | | | | |
| | HA2 | 53 ILE | QG1 | 6.5 | 2394.5 *2 | | HN | 52 ASN | HA | 4.1 | 29121 |
| 42 GLN | | | | | | | HN | 52 ASN | HB2 | 3.9 | 39020 |
| | HN | 42 GLN | HA | 4.3 | 22300 | | HN | 52 ASN | HB3 | 3.9 | 38560 |
| | HN | 59 TRP | HE1 | 5.5 | 23760 | | HN | 52 ASN | HD21 | 5.5 | 2924.1 |
| | HA | 43 ALA | HN | 5.5 | 4380 | | HN | 52 ASN | HD22 | 5.5 | 10130 |
| | HA | 45 GLY | HN | 5.5 | 2127.6 | | HN | 53 ILE | HN | 4.6 | 15438 |
| 43 ALA | | | | | | | HN | 55 LYS | QG | 6.5 | 22140 *2 |
| | HN | 43 ALA | HA | 3.2 | 101000 | | HA | 52 ASN | HB2 | 5.5 | 2093 |
| | HN | 43 ALA | QB | 3.6 | 149900 | | HA | 52 ASN | HD21 | 5.5 | 11673 |
| | HN | 44 GLU | HN | 5.1 | 9135 | | HA | 52 ASN | HD22 | 5.5 | 6783 |
| | HN | 45 GLY | HN | 5.5 | 3528 | | HA | 53 ILE | HN | 5.4 | 6849 |
| | HN | 48 TYR | CZ | 7.5 | 1691 *2 | | HA | 55 LYS | HN | 5.5 | 4844 |
| | HA | 43 ALA | QB | 3.5 | 187900 | | HA | 55 LYS | QB | 5.4 | 22030 *2 |
| | QB | 44 GLU | HN | 4 | 80690 | | HA | 55 LYS | QG | 6.5 | 16795 *2 |
| | QB | 44 GLU | HA | 4.8 | 40750 | | HA | 55 LYS | QD | 6.5 | 9805 *2 |
| | QB | 45 GLY | HN | 3.6 | 74280 | | HA | 57 VAL | HN | 5.5 | 2428 |
| | QB | 45 GLY | HA2 | 6.5 | 799 | | HB2 | 52 ASN | HD21 | 4.4 | 38600 |
| 44 GLU | | | | | | | HB2 | 52 ASN | HD22 | 5.5 | 10278 |
| | HN | 44 GLU | HA | 4.9 | 12090 | | HB2 | 53 ILE | HN | 5.3 | 8058 |
| | HN | 45 GLY | HN | 4.6 | 16820 | | HB3 | 52 ASN | HD21 | 3.7 | 96170 |
| | HN | 45 GLY | HA2 | 5.5 | 1258 | | HB3 | 52 ASN | HD22 | 5.5 | 13362 |
| | HA | 45 GLY | HN | 5.4 | 7037 | | HB3 | 53 ILE | HN | 4.5 | 17120 |
| 45 GLY | | | | | | | HD21 | 53 ILE | HA | 5.5 | 11070 |
| | HN | 45 GLY | HA1 | 4.2 | 26070 | | HD21 | 57 VAL | QG2 | 6.5 | 5725 |
| | HN | 45 GLY | HA2 | 3.4 | 79600 | | HD22 | 53 ILE | HA | 5.5 | 1113 |
| | HN | 48 TYR | CG | 7.5 | 1623.5 *2 | | HD22 | 57 VAL | QG2 | 6.5 | 2224 |
| | HN | 48 TYR | CZ | 7.5 | 4354 *2 | 53 ILE | | | | | |
| | HA2 | 48 TYR | CG | 7.5 | 9160 *2 | | HN | 53 ILE | HA | 3.8 | 42270 |
| | HA2 | 48 TYR | CZ | 7.5 | 20320 *2 | | HN | 53 ILE | HB | 3.2 | 105930 |
| 46 TYR | | | | | | | HN | 53 ILE | QG2 | 4.6 | 45770 |
| | HN | 46 TYR | HA | 3.7 | 48310 | | HN | 53 ILE | QG1 | 5.1 | 54200 *2 |
| | HN | 46 TYR | QB | 6 | 7140 *2 | | HN | 53 ILE | QD1 | 5.5 | 19260 |
| | HN | 46 TYR | HD1 | 3.1 | 255800 | | HN | 54 LYS | HN | 4.4 | 21060 |
| | HN | 48 TYR | CZ | 5.4 | 58300 *2 | | HN | 55 LYS | HN | 4.8 | 13470 |
| | HN | 49 THR | HN | 5.5 | 625 | | HN | 56 ASN | HA | 5.5 | 5313 |
| | HN | 49 THR | QG2 | 6.5 | 21740 | | HA | 53 ILE | QG2 | 5.4 | 21460 |
| | HA | 46 TYR | CG | 6.5 | 5590 *2 | | HA | 53 ILE | QG1 | 6.1 | 1494 *2 |
| | QB | 46 TYR | HD1 | 5.7 | 29830 *2 | | HA | 53 ILE | QD1 | 4.8 | 39350 |
| | QB | 46 TYR | HD2 | 6.1 | 19805 *2 | | HA | 54 LYS | HN | 5.4 | 7087 |
| | HD1 | 46 TYR | HE2 | 4 | 65310 | | HB | 53 ILE | QG1 | 4.5 | 122800 *2 |
| | HD1 | 49 THR | HN | 5.5 | 9494 | | HB | 53 ILE | QD1 | 3.3 | 520600 |
| | HD1 | 49 THR | QG2 | 5.1 | 70280 | | HB | 55 LYS | HN | 5.5 | 35.2 |
| | HD2 | 49 THR | HN | 5.5 | 1789 | | QG2 | 54 LYS | HN | 6.5 | 1382 |
| | HD2 | 49 THR | QG2 | 6.3 | 51180 | | QG2 | 54 LYS | HA | 6.5 | 961 |
| | HE2 | 49 THR | QG2 | 6.5 | 2864 | | QG1 | 54 LYS | HN | 6.5 | 2763 *2 |
| 48 TYR | | | | | | | QG1 | 54 LYS | HA | 6.5 | 21825 *2 |

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|---|---|---|---|---|---|
| | QD1 | 54 LYS | HN | 6.5 | 17847 |
| | QD1 | 54 LYS | HA | 6.5 | 31150 |
| 54 LYS | | | | | |
| | HN | 54 LYS | HA | 3.9 | 37530 |
| | HN | 54 LYS | HB2 | 3 | 134100 |
| | HN | 54 LYS | HB3 | 3.8 | 39570 |
| | HN | 54 LYS | HG2 | 5.5 | 4987 |
| | HN | 54 LYS | QG | 6 | 22005 *2 |
| | HN | 55 LYS | HN | 4.3 | 23880 |
| | HN | 55 LYS | QB | 6.5 | 1707 *2 |
| | HN | 56 ASN | HN | 5.3 | 7080 |
| | HN | 56 ASN | HA | 5.5 | 5898 |
| | HA | 54 LYS | HB2 | 3.7 | 50350 |
| | HA | 54 LYS | HB3 | 3.2 | 94860 |
| | HA | 54 LYS | QG | 5.1 | 34215 *2 |
| | HA | 55 LYS | HN | 5.5 | 5460 |
| | HB2 | 55 LYS | HN | 4.1 | 27620 |
| | QG | 55 LYS | HA | 6.5 | 2979 *2 |
| 55 LYS | | | | | |
| | HN | 55 LYS | HA | 4 | 30780 |
| | HN | 55 LYS | QB | 4.5 | 35295 *2 |
| | HN | 55 LYS | QG | 6.5 | 5890 *2 |
| | HN | 55 LYS | QD | 6.5 | 7835 *2 |
| | HN | 56 ASN | HN | 5.5 | 3048 |
| | HN | 57 VAL | QG2 | 6.5 | 1608 |
| | HA | 55 LYS | QB | 6.5 | 3500.5 *2 |
| | HA | 55 LYS | QG | 6.1 | 1768 *2 |
| | QB | 57 VAL | HN | 6.5 | 1934.5 *2 |
| | QB | 57 VAL | HB | 4.8 | 46755 *2 |
| | QB | 57 VAL | QG2 | 7.5 | 5280 *2 |
| | QG | 75 ILE | QG2 | 7.5 | 7445 *2 |
| 56 ASN | | | | | |
| | HN | 56 ASN | HA | 4 | 31980 |
| | HA | 57 VAL | HN | 4.2 | 25960 |
| | HA | 57 VAL | HB | 4.7 | 14640 |
| 57 VAL | | | | | |
| | HN | 57 VAL | HA | 3.8 | 43400 |
| | HN | 57 VAL | HB | 3.7 | 49530 |
| | HN | 57 VAL | QG1 | 4.9 | 33600 |
| | HN | 57 VAL | QG2 | 4.5 | 52540 |
| | HN | 58 LEU | HN | 5.5 | 4057 |
| | HA | 57 VAL | HB | 3.9 | 37580 |
| | HA | 57 VAL | QG1 | 4.6 | 47170 |
| | HA | 57 VAL | QG2 | 4.4 | 57420 |
| | HB | 57 VAL | QG1 | 3.9 | 114300 |
| | HB | 57 VAL | QG2 | 4.2 | 80500 |
| | HB | 59 TRP | HE1 | 5.5 | 4311 |
| | QG1 | 58 LEU | HN | 6.5 | 9420 |
| | QG1 | 59 TRP | HA | 6.5 | 5254 |
| | QG1 | 59 TRP | HD1 | 6.5 | 535 |
| | QG1 | 59 TRP | HE3 | 6.5 | 5117 |
| | QG1 | 59 TRP | HE1 | 6.5 | 1447 |
| | QG1 | 59 TRP | HZ3 | 6.5 | 1626 |
| | QG1 | 59 TRP | HZ2 | 6.5 | 5555 |
| | QG1 | 59 TRP | HH2 | 6.5 | 3755 |
| | QG2 | 58 LEU | HN | 6.5 | 3932 |
| | QG2 | 58 LEU | HB2 | 6.5 | 2711 |
| | QG2 | 58 LEU | QD2 | 7.5 | 1672 |
| | QG2 | 59 TRP | HN | 6.5 | 946 |
| | QG2 | 59 TRP | HA | 6.5 | 3514 |
| | QG2 | 59 TRP | HE3 | 6.5 | 8774 |
| | QG2 | 59 TRP | HE1 | 6.5 | 1764 |
| | QG2 | 59 TRP | HZ3 | 6.5 | 7208 |
| | QG2 | 59 TRP | HZ2 | 6.5 | 9734 |
| | QG2 | 75 ILE | QG2 | 7.5 | 7642 |
| 58 LEU | | | | | |
| | HN | 58 LEU | HA | 3.3 | 80650 |
| | HN | 58 LEU | HB2 | 4.5 | 18120 |
| | HN | 58 LEU | HB3 | 4.5 | 18000 |
| | HN | 58 LEU | HG | 5.5 | 5737 |
| | HN | 58 LEU | QD2 | 6.5 | 2035 |
| | HN | 59 TRP | HN | 4.9 | 11370 |
| | HA | 58 LEU | HB2 | 3.4 | 73660 |
| | HA | 58 LEU | HB3 | 4.5 | 18070 |
| | HA | 58 LEU | QD2 | 5.1 | 27270 |
| | HA | 59 TRP | HA | 5.5 | 6515 |
| | HA | 59 TRP | HD1 | 5.5 | 1134 |
| | HB2 | 58 LEU | QD1 | 4.6 | 48840 |
| | HB2 | 58 LEU | QD2 | 3.7 | 148200 |
| | HB2 | 59 TRP | HN | 5.5 | 5547 |
| | HB2 | 75 ILE | QG2 | 6.5 | 1910 |
| | HB3 | 58 LEU | QD1 | 4.7 | 42360 |
| | HB3 | 59 TRP | HN | 5.5 | 516 |
| | HG | 58 LEU | QD2 | 4.2 | 78160 |
| | QD1 | 59 TRP | HN | 6.5 | 22530 |
| | QD1 | 59 TRP | HA | 6.5 | 1439 |
| | QD1 | 59 TRP | HB3 | 4.2 | 96070 |
| | QD1 | 59 TRP | HD1 | 6.5 | 1275 |
| | QD1 | 59 TRP | HE3 | 6.5 | 19200 |
| | QD2 | 59 TRP | HN | 6.5 | 934 |
| | QD2 | 59 TRP | HE3 | 6.5 | 691 |
| 59 TRP | | | | | |
| | HN | 59 TRP | HA | 4.6 | 16440 |
| | HN | 59 TRP | HB2 | 4.5 | 17742 |
| | HN | 59 TRP | HB3 | 3.1 | 118900 |
| | HN | 59 TRP | HD1 | 5.5 | 11340 |
| | HN | 59 TRP | HE3 | 5.5 | 5500 |
| | HA | 59 TRP | HB2 | 5 | 10430 |
| | HA | 59 TRP | HE3 | 3.7 | 95540 |
| | HA | 59 TRP | HE1 | 5.5 | 176.2 |
| | HA | 60 ASP | HN | 5 | 10650 |
| | HB2 | 59 TRP | HD1 | 4.4 | 38730 |
| | HB2 | 59 TRP | HE3 | 5.5 | 13560 |
| | HB2 | 59 TRP | HE1 | 5.5 | 1245 |
| | HB3 | 59 TRP | HD1 | 4.9 | 22460 |
| | HB3 | 59 TRP | HE3 | 5.5 | 10670 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | HD1 | 59 TRP | HE1 | 4.3 | 44810 | | HB3 | 63 ASN | HD21 | 4.1 | 57780 |
| | HE3 | 59 TRP | HE1 | 5.5 | 10840 | | HB3 | 64 MET | HN | 5 | 10270 - |
| | HE3 | 59 TRP | HZ3 | 3.7 | 92200 | | HB3 | 64 MET | HB2 | 3.7 | 48420 |
| | HE3 | 59 TRP | HH2 | 5.5 | 3587 | | HB3 | 75 ILE | QD1 | 6.5 | 6014 |
| | HE3 | 60 ASP | HN | 5.5 | 8168 | | HD21 | 64 MET | HN | 5.5 | 14133 |
| | HE3 | 68 LEU | HG | 5.5 | 7084 | 64 THR | | | | | |
| | HE1 | 59 TRP | HZ3 | 5.5 | 3614 | | HN | 64 MET | HA | 4 | 34290 |
| | HE1 | 59 TRP | HZ2 | 5 | 21560 | | HN | 64 MET | HB2 | 5.5 | 3454 |
| | HZ3 | 59 TRP | HH2 | 4.2 | 51790 | | HN | 64 MET | HB3 | 3.6 | 54810 |
| | HZ3 | 67 TYR | HB2 | 5.2 | 26840 | | HN | 64 MET | QE | 6.1 | 11385 |
| | HZ3 | 67 TYR | HB3 | 5.5 | 24680 | | HN | 65 SER | HN | 4.6 | 15729 |
| | HZ3 | 68 LEU | HG | 5.5 | 3730 | | HN | 68 LEU | HG | 5.5 | 7221 |
| | HZ3 | 75 ILE | QD1 | 6.5 | 7707 | | HN | 75 ILE | HG12 | 5.5 | 1844.7 |
| | HZ2 | 59 TRP | HH2 | 4 | 66580 | | HA | 64 MET | HB2 | 5.5 | 6195 |
| | HZ2 | 75 ILE | HN | 5.5 | 10677 | | HA | 64 MET | HB3 | 4.3 | 21940 |
| | HZ2 | 75 ILE | HB | 3.9 | 43000 | | HA | 64 MET | QE | 6.1 | 11280 |
| | HZ2 | 75 ILE | QG2 | 6.5 | 913 | | HA | 67 TYR | HN | 5.5 | 2670 |
| | HH2 | 67 TYR | HB2 | 5.5 | 661 | | HA | 68 LEU | HN | 5.5 | 2935 |
| | HH2 | 67 TYR | HB3 | 5.5 | 2077 | | HB2 | 64 MET | QE | 4.9 | 33700 |
| 60 ASP | | | | | | | HB2 | 65 SER | HN | 4.8 | 12610 |
| | HN | 64 MET | HB2 | 5.5 | 4471 | | HB3 | 64 MET | QE | 5.8 | 15570 |
| | HN | 75 ILE | QG2 | 6.5 | 1573 | | HB3 | 65 SER | HN | 4.7 | 14322 |
| 62 ASN | | | | | | | HB3 | 65 SER | HA | 5.2 | 8454 |
| | HN | 62 ASN | HA | 3.7 | 47370 | | HB3 | 68 LEU | QD1 | 5 | 72040 |
| | HN | 62 ASN | HB2 | 4.8 | 13060 | | QE | 65 SER | HN | 6.5 | 1667.4 |
| | HN | 62 ASN | HB3 | 3.7 | 45810 | | QE | 95 ILE | QG1 | 7.5 | 2275.5 *2 |
| | HN | 63 ASN | HN | 5.5 | 985.2 | 65 ASN | | | | | |
| | HN | 63 ASN | HA | 5.5 | 2095 | | HN | 65 SER | HA | 4.2 | 24426 |
| | HN | 63 ASN | HB3 | 5.5 | 968 | | HN | 65 SER | HB2 | 3.7 | 46560 |
| | HN | 63 ASN | HD21 | 5.5 | 5268 | | HN | 65 SER | HB3 | 3.9 | 38730 |
| | HN | 64 MET | HB3 | 5.5 | 3962 | | HN | 66 GLU | HN | 4.5 | 18470 |
| | HN | 75 ILE | HG12 | 5.5 | 23457 | | HA | 65 SER | HB2 | 4.8 | 12500 |
| | HN | 75 ILE | HG13 | 5.5 | 10008 | | HA | 66 GLU | HN | 5.5 | 2316 |
| | HA | 63 ASN | HN | 5.5 | 4380 | | HA | 68 LEU | HB2 | 5.5 | 1446 |
| | HB2 | 63 ASN | HN | 4.9 | 11140 | | HA | 68 LEU | QD1 | 6.5 | 2766 |
| | HB3 | 63 ASN | HN | 5.5 | 6756 | | HA | 91 ARG | HB2 | 5.5 | 1351 |
| 63 ASN | | -5 | | | | | HA | 91 ARG | QG | 6.5 | 1093 *2 |
| | HN | 63 ASN | HA | 3.3 | 91500 | | HB2 | 66 GLU | HN | 4.9 | 12070 |
| | HN | 63 ASN | HB2 | 5.5 | 711 | 66 GLU | | | | | |
| | HN | 63 ASN | HB3 | 4.5 | 17367 | | HN | 66 GLU | HA | 4.1 | 28314 |
| | HN | 63 ASN | HD21 | 4.6 | 30660 | | HN | 66 GLU | HB2 | 3.4 | 69480 |
| | HN | 63 ASN | HD22 | 5.5 | 4983 | | HN | 66 GLU | HB3 | 4 | 30930 |
| | HN | 64 MET | HN | 4.8 | 12903 | | HN | 66 GLU | QG | 6.5 | 6460 *2 |
| | HN | 64 MET | HA | 5.5 | 192.9 | | HN | 67 TYR | HN | 4.1 | 29907 |
| | HN | 64 MET | HB2 | 5.5 | 5099 | | HN | 68 LEU | HN | 5.5 | 5403 |
| | HN | 75 ILE | HG12 | 5.5 | 2026 | | HA | 66 GLU | HB2 | 4.3 | 22280 |
| | HN | 75 ILE | QD1 | 6.5 | 1039 | | HA | 66 GLU | HB3 | 4.4 | 20370 |
| | HA | 63 ASN | HB3 | 3.5 | 61600 | | HA | 66 GLU | QG | 6.1 | 720.5 *2 |
| | HA | 63 ASN | HD21 | 4.1 | 60170 | | HA | 67 TYR | HN | 5.5 | 2496 |
| | HA | 63 ASN | HD22 | 4.9 | 24370 | | HB2 | 66 GLU | QG | 4.4 | 146750 *2 |
| | HA | 64 MET | HN | 4.4 | 20037 | | HB2 | 67 TYR | HN | 4.2 | 25210 |
| | HA | 66 GLU | HB2 | 5.5 | 738 | | HB3 | 67 TYR | HN | 4.1 | 28599 |
| | HA | 67 TYR | HN | 5.5 | 628 | 67 TYR | | | | | |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | HN | 67 TYR | HA | 4.1 | 29990 | | HA | 71 PRO | HB2 | 3.8 | 44480 |
| | HN | 67 TYR | HB2 | 3.6 | 57870 | | HA | 71 PRO | HB3 | 3.6 | 53380 |
| | HN | 67 TYR | HB3 | 3.8 | 45030 | | HA | 71 PRO | QG | 6.1 | 5155 *2 |
| | HN | 68 LEU | HA | 5.5 | 357 | | HA | 71 PRO | QD | 6.4 | 13980 *2 |
| | HN | 68 LEU | HB2 | 5 | 10053 | | HA | 73 LYS | HN | 5.5 | 2904 |
| | HN | 68 LEU | HG | 5.5 | 441 | | HA | 73 LYS | HG2 | 4.6 | 33250 |
| | HA | 67 TYR | HB2 | 5.5 | 651 | | HA | 85 LEU | HG | 5.5 | 8961 |
| | HA | 67 TYR | HB3 | 3.6 | 55700 | | HA | 85 LEU | QD1 | 6.5 | 7771 |
| | HA | 68 LEU | HN | 5.4 | 6894 | | HB2 | 73 LYS | HG2 | 5.5 | 1113 |
| | HB3 | 68 LEU | HN | 3.8 | 40010 | | HB2 | 82 PHE | CZ | 7.5 | 1387.5 *2 |
| 68 LEU | | | | | | | HB2 | 82 PHE | HZ | 5.5 | 3505 |
| | HN | 68 LEU | HA | 3.4 | 69750 | | HB3 | 72 ALA | HN | 5.5 | 4631 |
| | HN | 68 LEU | HB2 | 3.4 | 71730 | | HB3 | 73 LYS | HN | 5.5 | 1185 |
| | HN | 68 LEU | HB3 | 3.9 | 37400 | | HB3 | 73 LYS | HG2 | 5.5 | 9423 |
| | HN | 68 LEU | HG | 4.1 | 55200 | | HB3 | 82 PHE | HZ | 5.5 | 1737 |
| | HN | 68 LEU | QD1 | 5.6 | 17440 | 72 ALA | | | | | |
| | HN | 69 THR | HN | 4.3 | 21660 | | HN | 73 LYS | HN | 5.4 | 6900 |
| | HN | 91 ARG | QG | 6.5 | 11590 *2 | | HN | 73 LYS | HA | 5.5 | 645 |
| | HA | 68 LEU | HB2 | 5.5 | 349 | | HN | 73 LYS | HG2 | 5.5 | 2015 |
| | HA | 68 LEU | HB3 | 5.5 | 4987 | | HN | 82 PHE | CG | 5.1 | 69950 *2 |
| | HA | 68 LEU | HG | 5.5 | 6548 | | HN | 82 PHE | CZ | 7.5 | 16140 *2 |
| | HA | 68 LEU | QD1 | 3.8 | 119500 | 73 LYS | | | | | |
| | HA | 69 THR | HN | 4.6 | 15200 | | HB2 | 73 LYS | QD | 5 | |
| | HA | 91 ARG | QG | 6.5 | 1372 *2 | | HB3 | 73 LYS | QD | 5 | |
| | HB2 | 68 LEU | HG | 2.6 | 583500 | | HN | 73 LYS | HA | 5.5 | 5979 |
| | HB2 | 68 LEU | QD1 | 4.1 | 89850 | | HN | 73 LYS | HB3 | 4.1 | 28850 |
| | HB2 | 69 THR | HN | 5.5 | 2655 | | HN | 73 LYS | HG2 | 5.5 | 3588 |
| | HB2 | 91 ARG | QG | 6.1 | 27635 *2 | | HB2 | 73 LYS | HG2 | 5.5 | 213 |
| | HB3 | 68 LEU | HG | 3.4 | 138600 | | HB3 | 73 LYS | HG2 | 5.5 | 898 |
| | HB3 | 68 LEU | QD1 | 4.9 | 34130 | | HB3 | 82 PHE | QB | 6.5 | 756 *2 |
| | HB3 | 69 THR | HN | 5.2 | 8791 | 75 ILE | | | | | |
| | HB3 | 91 ARG | HN | 5.5 | 2114 | | HN | 75 ILE | HA | 3.5 | 66750 |
| | HB3 | 91 ARG | HA | 5.5 | 3121 | | HN | 75 ILE | HB | 4.4 | 19683 |
| | HG | 68 LEU | QD1 | 3.5 | 179200 | | HN | 75 ILE | QG2 | 5.9 | 13900 |
| | HG | 75 ILE | HN | 5.4 | 25380 | | HN | 75 ILE | HG12 | 4.3 | 46170 |
| | HG | 75 ILE | QD1 | 6.5 | 763 | | HN | 75 ILE | HG13 | 4.7 | 29360 |
| | QD1 | 69 THR | HN | 6.5 | 5553 | | HN | 75 ILE | QD1 | 5.6 | 17280 |
| | QD1 | 75 ILE | QD1 | 7.5 | 4898 | | HA | 75 ILE | QG2 | 3.8 | 127500 |
| | QD1 | 91 ARG | QG | 7.5 | 29270 *2 | | HA | 75 ILE | QD1 | 6.5 | 8088 |
| | QD1 | 94 LEU | QD2 | 7.5 | 27820 | | HB | 75 ILE | QG2 | 4.4 | 61260 |
| | QD1 | 95 ILE | QG1 | 7.5 | 2334.5 *2 | | HB | 75 ILE | QD1 | 5.4 | 21370 |
| | QD1 | 95 ILE | QD1 | 7.5 | 4116 | | QG2 | 75 ILE | HG12 | 3.9 | 112900 |
| 69 THR | | | | | | | QG2 | 75 ILE | HG13 | 4.2 | 80290 |
| | HN | 69 THR | HA | 4.2 | 24294 | | QG2 | 75 ILE | QD1 | 4.4 | 226900 |
| | HN | 69 THR | HB | 3.7 | 48030 | | HG12 | 75 ILE | QD1 | 3.9 | 110400 |
| | HN | 69 THR | QG2 | 6.1 | 11520 | | HG13 | 75 ILE | QD1 | 4.1 | 81360 |
| | HN | 70 ASN | HN | 3.9 | 35910 | 79 ALA | | | | | |
| | HA | 70 ASN | HN | 5.5 | 6135 | | HN | 79 ALA | HA | 4.6 | 16650 |
| 70 ASN | | | | | | | HN | 79 ALA | QB | 3.8 | 112400 |
| | HN | 70 ASN | HA | 3.6 | 57660 | | HN | 80 MET | HN | 5.5 | 3044 |
| | HN | 70 ASN | HB2 | 3.9 | 37530 | | HN | 80 MET | HA | 5.5 | 6153 |
| | HN | 70 ASN | HB3 | 4.7 | 13953 | | HN | 80 MET | HG2 | 5.5 | 1822.2 |
| 71 PRO | | | | | | | HA | 79 ALA | QB | 3.8 | 119600 |

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|---|---|---|---|---|---|
| | HA | 80 MET | HN | 5.5 | 1114.8 |
| | QB | 80 MET | HN | 5.6 | 10960 |
| 80 MET | | | | | |
| | HN | 80 MET | HA | 5.1 | 9772 |
| | HN | 80 MET | HG2 | 4.6 | 30870 |
| | HN | 80 MET | HG3 | 5.5 | 6162 |
| | HN | 80 MET | QE | 5.2 | 25700 |
| | HN | 81 ALA | HN | 3.7 | 48340 |
| | HN | 81 ALA | HA | 4.6 | 16170 |
| | HN | 81 ALA | QB | 6.5 | 550.5 |
| | HA | 80 MET | QE | 5.7 | 15810 |
| | HA | 81 ALA | HN | 5.5 | 6549 |
| | HG2 | 80 MET | QE | 3.3 | 271800 |
| | HG2 | 84 GLY | HN | 5.2 | 27249 |
| | HG3 | 80 MET | QE | 4.2 | 75640 |
| | QE | 81 ALA | HN | 6.5 | 6168 |
| | QE | 83 GLY | HN | 6.5 | 12940 |
| | QE | 84 GLY | HN | 6.5 | 12591 |
| 81 ALA | | | | | |
| | HN | 81 ALA | HA | 4.6 | 15230 |
| | HN | 81 ALA | QB | 4.5 | 39810 |
| | HN | 83 GLY | HN | 5.5 | 1608.9 |
| | HA | 81 ALA | QB | 4.8 | 28130 |
| | QB | 83 GLY | HN | 6.5 | 518.1 |
| 82 PHE | | | | | |
| | QB | 82 PHE | CG | 8.5 | 7117.5 *4 |
| | QB | 82 PHE | HZ | 6.5 | 1897 *2 |
| | CG | 82 PHE | CZ | 8.1 | 58600 *4 |
| | CG | 82 PHE | HZ | 6.7 | 29470 *2 |
| | CG | 85 LEU | HN | 7.5 | 7740 *2 |
| | CZ | 82 PHE | HZ | 5.6 | 113950 *2 |
| | CZ | 85 LEU | HN | 7.5 | 10791 *2 |
| | CZ | 85 LEU | HB2 | 7.5 | 14595 *2 |
| | CZ | 85 LEU | QD1 | 8.5 | 14680 *2 |
| | HZ | 85 LEU | HB2 | 5.5 | 14660 |
| | HZ | 85 LEU | QD1 | 6.5 | 8509 |
| 83 GLY | | | | | |
| | HN | 84 GLY | HN | 5.5 | 3795 |
| | HN | 84 GLY | HA1 | 5.5 | 4770 |
| | HN | 85 LEU | HB3 | 5.5 | 1753.2 |
| 84 GLY | | | | | |
| | HN | 84 GLY | HA1 | 4.3 | 21744 |
| | HN | 85 LEU | HN | 3.5 | 60150 |
| | HN | 85 LEU | HB3 | 5.5 | 1548 |
| 85 LEU | | | | | |
| | HN | 85 LEU | HA | 3.5 | 63300 |
| | HN | 85 LEU | HB2 | 4.1 | 28707 |
| | HN | 85 LEU | HB3 | 4.4 | 20322 |
| | HN | 85 LEU | HG | 4.2 | 50830 |
| | HN | 85 LEU | QD1 | 6 | 12945 |
| | HN | 86 LYS | HN | 4.1 | 29946 |
| | HB2 | 85 LEU | QD1 | 4.3 | 68590 |
| | HB2 | 86 LYS | HN | 3.5 | 59880 |
| | HB2 | 87 LYS | HN | 5.5 | 1827.9 |
| | HG | 86 LYS | QE | 6.5 | 10660 *2 |
| 86 LYS | | | | | |
| | HN | 86 LYS | HA | 5.5 | 4158 |
| | HN | 86 LYS | QG | 5.3 | 46515 *2 |
| | HN | 86 LYS | HD2 | 5.4 | 14808 |
| | HN | 86 LYS | HD3 | 5.1 | 19767 |
| | HN | 86 LYS | QE | 6 | 20265 *2 |
| | HN | 87 LYS | HN | 3.6 | 55980 |
| | QG | 87 LYS | HN | 6.5 | 15615 *2 |
| | HD3 | 86 LYS | QE | 5.6 | 32565 *2 |
| 87 LYS | | | | | |
| | HN | 87 LYS | HA | 4.1 | 28314 |
| | HN | 87 LYS | HB2 | 4.3 | 22653 |
| | HN | 87 LYS | HB3 | 4.4 | 19308 |
| | HN | 87 LYS | QG | 6 | 21450 *2 |
| | HN | 87 LYS | QD | 4.9 | 70980 *2 |
| | HN | 87 LYS | QE | 6.5 | 5959.5 *2 |
| 90 ASP | | | | | |
| | HN | 90 ASP | HA | 5.5 | 2797.8 |
| | HN | 90 ASP | HB2 | 4.4 | 19461 |
| | HN | 90 ASP | HB3 | 4.1 | 29166 |
| | HN | 91 ARG | HN | 4.3 | 22371 |
| | HN | 91 ARG | HB3 | 4.3 | 21600 |
| | HN | 91 ARG | QG | 6.5 | 1432.8 *2 |
| | HN | 92 ASN | HN | 5.5 | 1331.1 |
| | HA | 90 ASP | HB2 | 4.9 | 12250 |
| | HA | 90 ASP | HB3 | 5.5 | 5477 |
| | HA | 91 ARG | HN | 5.5 | 3317 |
| | HA | 92 ASN | HN | 5.5 | 498.3 |
| | HA | 93 ASP | HN | 5.5 | 1847.4 |
| | HB2 | 91 ARG | HN | 5.2 | 8973 |
| | HB2 | 91 ARG | HB2 | 5.3 | 26470 |
| | HB3 | 91 ARG | HN | 4.7 | 14784 |
| 91 ARG | | | | | |
| | HN | 91 ARG | HA | 4.6 | 16308 |
| | HN | 91 ARG | HB2 | 3.9 | 38610 |
| | HN | 91 ARG | HB3 | 4.5 | 17064 |
| | HN | 91 ARG | QG | 6.4 | 14671.5 *2 |
| | HN | 92 ASN | HN | 4.3 | 22887 |
| | HN | 92 ASN | QB | 6.5 | 1754.5 *2 |
| | HN | 93 ASP | HN | 5.5 | 523.2 |
| | HN | 94 LEU | HB3 | 5.5 | 3819 |
| | HA | 92 ASN | HN | 5.5 | 5044 |
| | HA | 94 LEU | HN | 5.5 | 3048 |
| | HA | 94 LEU | HB3 | 5.5 | 642 |
| | HA | 94 LEU | HG | 5.5 | 23990 |
| | HA | 94 LEU | QD2 | 6.5 | 30250 |
| | HA | 95 ILE | HN | 5.2 | 8120 |
| | HA | 95 ILE | QD1 | 6.5 | 35620 |
| | HB2 | 92 ASN | HN | 5.4 | 7143 |
| | HB3 | 92 ASN | HN | 5.1 | 9912 |
| | HB3 | 94 LEU | HN | 5.5 | 2195 |

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|---|---|---|---|---|---|
| | QG | 92 ASN | HN | 6.5 | 1091.2 *2 |
| 92 ASN | | | | | |
| | HN | 92 ASN | HA | 3.9 | 35910 |
| | HN | 92 ASN | QB | 4.7 | 30400 *2 |
| | HN | 94 LEU | HN | 4.2 | 29930 |
| | HA | 92 ASN | QB | 6.1 | 841 *2 |
| | HA | 93 ASP | HN | 4.8 | 13113 |
| | HA | 95 ILE | HN | 5.5 | 3442 |
| | HA | 95 ILE | QG1 | 6.5 | 4499.5 *2 |
| | HA | 95 ILE | QD1 | 6.5 | 369 |
| | HA | 96 THR | HN | 4.9 | 12750 |
| | QB | 93 ASP | HN | 6.3 | 7540.5 *2 |
| | QB | 93 ASP | HA | 6.5 | 2321.5 *2 |
| | QB | 95 ILE | QG2 | 7.5 | 1159 *2 |
| 93 ASP | | | | | |
| | HN | 93 ASP | HA | 4.2 | 24726 |
| | HN | 93 ASP | QB | 5.3 | 14394 *2 |
| | HN | 94 LEU | HN | 4 | 34330 |
| | HA | 94 LEU | HN | 5.5 | 3630 |
| | HA | 96 THR | HN | 3.8 | 52510 |
| | HA | 97 TYR | HN | 4.9 | 11390 |
| | QB | 94 LEU | HN | 5.4 | 18960 *2 |
| | QB | 95 ILE | HN | 6.5 | 4981.5 *2 |
| 94 LEU | | | | | |
| | HN | 94 LEU | HA | 4.2 | 24678 |
| | HN | 94 LEU | HB2 | 3.6 | 58380 |
| | HN | 94 LEU | HB3 | 3.3 | 84250 |
| | HN | 94 LEU | HG | 5.5 | 11496 |
| | HN | 94 LEU | QD2 | 6.2 | 10668 |
| | HN | 95 ILE | HN | 3.8 | 43530 |
| | HA | 94 LEU | HG | 4.4 | 41150 |
| | HA | 95 ILE | HN | 5.5 | 5205 |
| | HA | 96 THR | HN | 5.5 | 5730 |
| | HA | 97 TYR | HN | 5 | 10089 |
| | HA | 97 TYR | HB3 | 5.5 | 4344 |
| | HA | 98 LEU | HN | 5.5 | 1509 |
| | HA | 98 LEU | HG | 5.5 | 18980 |
| | HA | 98 LEU | QD1 | 6.5 | 640 |
| | HB2 | 94 LEU | QD2 | 3.3 | 843400 |
| | HB2 | 95 ILE | HN | 4.4 | 20140 |
| | HB3 | 94 LEU | HG | 5 | 20180 |
| | HB3 | 94 LEU | QD2 | 4.4 | 62420 |
| | HB3 | 95 ILE | HN | 4.4 | 20900 |
| | HB3 | 95 ILE | HA | 5.5 | 573 |
| | HG | 95 ILE | HN | 5.5 | 1209 |
| | HG | 98 LEU | QD2 | 6.5 | 4003 |
| | QD2 | 95 ILE | HN | 6.5 | 12060 |
| | QD2 | 98 LEU | HN | 6.5 | 7014 |
| | QD2 | 98 LEU | HB2 | 3.3 | 219100 |
| 95 ILE | | | | | |
| | HN | 95 ILE | HA | 3.2 | 103800 |
| | HN | 95 ILE | HB | 3.2 | 96030 |
| | HN | 95 ILE | QG2 | 6.2 | 10840 |
| | HN | 95 ILE | QG1 | 5.8 | 25630 *2 |
| | HN | 95 ILE | QD1 | 6.4 | 9191 |
| | HN | 96 THR | HN | 4.8 | 12465 |
| | HN | 96 THR | QG2 | 6.5 | 2180.1 |
| | HN | 97 TYR | HN | 5.5 | 4749 |
| | HN | 98 LEU | HN | 4.8 | 13790 |
| | HA | 95 ILE | QG1 | 6.1 | 7420 *2 |
| | HA | 95 ILE | QD1 | 6.5 | 4350 |
| | HA | 96 THR | HN | 5.4 | 6905 |
| | HA | 98 LEU | HN | 5.5 | 476 |
| | HA | 98 LEU | QD2 | 6.5 | 2498 |
| | HA | 99 LYS | HN | 5.2 | 8011 |
| | HB | 96 THR | HN | 4.4 | 18990 |
| | QG2 | 95 ILE | QD1 | 7.5 | 1375 |
| | QG2 | 98 LEU | HB2 | 6.5 | 5709 |
| | QG2 | 98 LEU | QD1 | 7.5 | 34680 |
| | QG2 | 99 LYS | QD | 7.5 | 7310 *2 |
| | QG1 | 95 ILE | QD1 | 4.7 | 146700 *2 |
| | QG1 | 96 THR | HN | 6.5 | 1041.5 *2 |
| | QG1 | 98 LEU | HB2 | 4 | 72750 *2 |
| | QD1 | 96 THR | HN | 6.5 | 3604 |
| | QD1 | 98 LEU | QD1 | 4.3 | 192500 |
| 96 THR | | | | | |
| | HN | 96 THR | HA | 4.1 | 27220 |
| | HN | 96 THR | HB | 3.2 | 95280 |
| | HN | 96 THR | QG2 | 5.3 | 23859 |
| | HN | 97 TYR | HN | 3.4 | 71880 |
| | HN | 97 TYR | HA | 5.5 | 4554 |
| | HN | 99 LYS | HN | 5.5 | 1416.3 |
| | HA | 96 THR | HB | 5.5 | 957 |
| | HA | 96 THR | QG2 | 6 | 12820 |
| | HA | 97 TYR | HN | 5 | 10010 |
| | HA | 99 LYS | HN | 5.5 | 2901 |
| | HA | 99 LYS | HB2 | 5.5 | 1929 |
| | HB | 97 TYR | HN | 4.5 | 18460 |
| | QG2 | 97 TYR | HN | 6.5 | 9007 |
| 97 TYR | | | | | |
| | HN | 97 TYR | HA | 3.7 | 47250 |
| | HN | 97 TYR | HB2 | 3.9 | 36570 |
| | HN | 97 TYR | HB3 | 3.9 | 36150 |
| | HN | 98 LEU | HN | 4.4 | 21234 |
| | HN | 98 LEU | HA | 5.5 | 1289 |
| | HN | 98 LEU | HB2 | 5.5 | 841 |
| | HN | 99 LYS | QB | 6.5 | 3510 *2 |
| | HA | 97 TYR | HB2 | 5.5 | 1556 |
| | HA | 97 TYR | HB3 | 5.1 | 9590 |
| | HA | 98 LEU | HN | 5.4 | 6942 |
| | HA | 100 LYS | QB | 4.8 | 59300 *2 |
| | HB2 | 98 LEU | HN | 4.2 | 25910 |
| | HB3 | 98 LEU | HN | 4.5 | 18320 |
| | HB3 | 98 LEU | HB2 | 5.5 | 1914 |
| | HB3 | 98 LEU | HB3 | 5.5 | 12940 |
| | HB3 | 98 LEU | QD2 | 6.5 | 1864 |

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|---|---|---|---|---|---|---|
| 98 LEU | | | | | | |
| | HN | 98 LEU | HA | 4.1 | 28060 | |
| | HN | 98 LEU | HB2 | 3.9 | 38520 | |
| | HN | 98 LEU | HB3 | 4.1 | 27430 | |
| | HN | 98 LEU | QB | 4.5 | 34890 | *2 |
| | HN | 98 LEU | HG | 4.9 | 22910 | |
| | HN | 98 LEU | QD1 | 5.7 | 15774 | |
| | HN | 98 LEU | QD2 | 6.5 | 1707 | |
| | HN | 99 LYS | HN | 4.7 | 14742 | |
| | HN | 99 LYS | QB | 6.5 | 416 | *2 |
| | HN | 99 LYS | QD | 6.5 | 605.5 | *2 |
| | HA | 98 LEU | HB2 | 5.5 | 4083 | |
| | HA | 98 LEU | HB3 | 5.5 | 2942 | |
| | HA | 98 LEU | HG | 4.7 | 27640 | |
| | HA | 98 LEU | QD1 | 5 | 32300 | |
| | HA | 98 LEU | QD2 | 6.5 | 947 | |
| | HA | 99 LYS | HN | 5.5 | 4737 | |
| | HA | 99 LYS | QD | 6.5 | 13025 | *2 |
| | HA | 100 LYS | HN | 5.5 | 2348 | |
| | HA | 101 ALA | HN | 5 | 10860 | |
| | HA | 101 ALA | QB | 4 | 43450 | |
| | HA | 102 THR | HN | 5.5 | 5383 | |
| | HB2 | 98 LEU | QD1 | 4.2 | 74200 | |
| | HB2 | 98 LEU | QD2 | 6.5 | 839 | |
| | HB2 | 99 LYS | HN | 5.5 | 6463 | |
| | HB2 | 99 LYS | HA | 5.5 | 2496 | |
| | HB2 | 99 LYS | QD | 4.6 | 52350 | *2 |
| | HB2 | 102 THR | HN | 5.5 | 3189 | |
| | HB3 | 98 LEU | QD1 | 4.2 | 74970 | |
| | HB3 | 98 LEU | QD2 | 6.5 | 2231 | |
| | HB3 | 99 LYS | QD | 5 | 41995 | *2 |
| | HB3 | 102 THR | HN | 5.5 | 4553 | |
| | QB | 99 LYS | HN | 6.5 | 6507 | *2 |
| | HG | 98 LEU | QD1 | 3.8 | 134000 | |
| | HG | 99 LYS | HN | 5.5 | 15310 | |
| | QD1 | 99 LYS | HN | 6.5 | 8919 | |
| 99 LYS | | | | | | |
| | HN | 99 LYS | HA | 4.2 | 26211 | |
| | HN | 99 LYS | QB | 5.2 | 16915 | *2 |
| | HN | 99 LYS | QG | 6.5 | 9430 | *2 |
| | HN | 99 LYS | QD | 6.4 | 14155.5 | *2 |
| | HN | 100 LYS | HN | 4.1 | 28374 | |
| | HN | 100 LYS | QB | 6.5 | 764.5 | *2 |
| | HN | 100 LYS | QG | 6.2 | 26950 | *2 |
| | HN | 101 ALA | HN | 5.5 | 5712 | |
| | HA | 99 LYS | QB | 5.8 | 12640 | *2 |
| | HA | 99 LYS | QG | 6.1 | 6785 | *2 |
| | HA | 100 LYS | HN | 5.1 | 9161 | |
| | HA | 103 GLU | HN | 4.7 | 15250 | |
| | HA | 103 GLU | HB3 | 5.5 | 564 | |
| | HB2 | 100 LYS | HN | 4.4 | 21075 | |
| | QB | 100 LYS | HN | 5.8 | 12620 | *2 |
| | QG | 100 LYS | HN | 6.5 | 5022 | *2 |
| | QD | 100 LYS | HN | 6.5 | 3328 | *2 |
| | QD | 103 GLU | HN | 6.5 | 3370.5 | *2 |
| | QD | 103 GLU | HB3 | 3.4 | 123450 | *2 |
| 100 LYS | | | | | | |
| | HN | 100 LYS | HA | 3.8 | 41490 | |
| | HN | 100 LYS | QB | 4.4 | 40885 | *2 |
| | HN | 100 LYS | QG | 6 | 20385 | *2 |
| | HN | 101 ALA | HN | 3.7 | 48620 | |
| | HN | 101 ALA | QB | 6.5 | 2589 | |
| | HN | 102 THR | HN | 5.5 | 1362 | |
| | HA | 100 LYS | QB | 4.4 | 79550 | *2 |
| | HA | 101 ALA | HN | 5.4 | 6813 | |
| | HA | 103 GLU | HN | 5.5 | 3192 | |
| | HA | 103 GLU | HB3 | 5.1 | 9421 | |
| | QB | 101 ALA | HN | 5.2 | 25995 | *2 |
| | QG | 101 ALA | HN | 6.5 | 3352 | *2 |
| | QG | 101 ALA | HA | 6.5 | 11475 | *2 |
| 101 ALA | | | | | | |
| | HN | 101 ALA | HA | 4.1 | 27990 | |
| | HN | 101 ALA | QB | 3.9 | 95000 | |
| | HN | 102 THR | HN | 4.5 | 17376 | |
| | HA | 101 ALA | QB | 3.4 | 223000 | |
| | HA | 102 THR | HN | 5.1 | 9737 | |
| | HA | 103 GLU | HN | 5.5 | 4557 | |
| | QB | 102 THR | HN | 5.6 | 11040 | |
| 102 THR | | | | | | |
| | HN | 102 THR | HA | 5 | 10030 | |
| | HN | 102 THR | QG2 | 5 | 33040 | |
| | HN | 103 GLU | HN | 4.2 | 25780 | |
| | HN | 103 GLU | HB3 | 5.5 | 45.6 | |
| | HA | 102 THR | QG2 | 4.5 | 54520 | |
| | HA | 103 GLU | HN | 4.5 | 17829 | |
| | HA | 103 GLU | HB3 | 5.5 | 651 | |
| 103 GLU | | | | | | |
| | HN | 103 GLU | HA | 3.1 | 113100 | |
| | HN | 103 GLU | HB2 | 3.8 | 43890 | |
| | HN | 103 GLU | HB3 | 2.8 | 203850 | |
| | HN | 103 GLU | QG | 6.5 | 7490 | *2 |
| | HA | 103 GLU | HB2 | 5.5 | 143 | |
| | HA | 103 GLU | HB3 | 5.5 | 312 | |

**H-bond restraints for structure calculations**:

His18 Hδ1 - Pro30 O upper limit: 2.4 Å

His18 Nδ1 - Pro30 O lower limit=2.7 Å, upper limit: 3.4 Å